TESIS DOCTORAL/DOKTOREGO TESIA

Equilibrium and Transport Properties of Quantum Many-Body Systems

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DOCTORAL THESIS

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Abstract

This thesis is a study of equilibrium and dynamical properties of macroscopic quantum many-body problems. An important part of the manuscript concerns the study of heat and charge transport properties of fermions on the lattice. This refers to the derivation, from first principles of quantum mechanics and thermodynamics, of Ohm's law, first published in 1827 by *G. S. Ohm* [1], and of the heat equation, the well-known (classical) equation introduced by *J. Fourier* in 1807 [2]. A complete derivation of the heat equation from quantum mechanics is still not achieved, but we prove here some preliminary results on this non-trivial issue. By contrast, the study of charge transport properties of fermion systems on the lattice is largely developed in this thesis. This is an important issue of Physics, since, in recent history, the growing need for smaller electronic components has increased the interest in studying conductivity theory at atomic scale. The classical law of conductivity in material is Ohm's law. It is an empirical observation saying that the voltage on a conducting material is linearly proportional to the current flowing through it, the corresponding linear coefficient, i.e., the resistance, being growing linearly with respect to the length of the conducting sample. While it was expected that this classical behavior would break down at the microscopic scale where quantum effect dominates, in 2012 (see [58]), *B. Weber et al.* constructed atomic-scale nanowires in Si and observed that Ohm's law remains valid. Their experimental measurements of electric resistance demonstrate that quantum effects on charge transport almost disappear for nanowires of lengths larger than a few nanometers, even at very low temperatures ($4.2K$). In this thesis, we mathematically reinforce this observation by showing, for non-interacting (or quasi-free) lattice fermions in a (very general) disordered media (initially) at equilibrium that quantum uncertainty of microscopic electric current density around their (classical) macroscopic values is suppressed exponentially fast with respect to the volume of the region of the lattice where an external electric field is applied. This is in accordance with the above experimental observation. This result is a continuation of a series of articles recently published, for instance [34, 29], where the authors showed the convergence of the expectation values of microscopic current densities, the rate of convergence being however not studied in this series of papers.

Note that the equilibrium states on which transport properties are studied refer to KMS states, an elegant notion of equilibrium introduced by *R. Kubo*, *P.C. Martin* and *J. Schwinger* at the end of 50's. Such KMS states are of course not only defined for fermion systems, but for general ones. They are just products of the 2^{nd} law of thermodynamics, as shown in 1978 by *W. Pusz* and *S.L. Woronowicz* in [52]. Here, we study the consequence of the (quantum) KMS condition for a many-*boson* system on the lattice in the semiclassical limit. We prove that the classical KMS condition can be derived from the (quantum) KMS one for the Bose-Hubbard dynamical system on a finite graph.

Thesis Plan

Chapter 1 is aimed to give first intuitions to the reader on the formulation of quantum mechanics. In particular, we introduce the algebraic formulation of quantum mechanics where the Hilbert space structure is not anymore a backbone of the framework. Nevertheless, we recall the link between the algebraic formulation and the Hilbert space formulation at the end of the chapter.
In Chapter 2, we explain a well-known concept of equilibrium state which is fundamental in this thesis. Indeed, all the systems considered here are initially in the equilibrium state. In order to define the equilibrium state, one can, for instance, use a variational problem corresponding to minimize the free-energy entropy. Here, we rely on the notion of KMS state, which is related to the 2^{nd} law of thermodynamics and the so-called complete passiveness of an equilibrium state. The 2^{nd} law originates in *N.L.S Carnot*'s work in the 19^{th} century, and this is still used nowadays through mathematical works of *E.H. Lieb*, *J. Yngvason* or other researchers such as *W. Pusz*, *S.L. Woronowicz*, *J.B. Bru* and *W. de Siqueira Pedra*.
In Chapter 3, we introduce the algebraic formulation of quantum many-body problems. A standard framework to understand this construction is the well-known Fock space, which will be explained for pedagogical reasons. Because of the distinction between fermions and bosons, we develop the two different ways for the algebraic formulation of quantum many-body problems.
Chapter 4 gathers the tools directly used in order to formulate properly the results that we obtained during the thesis on transport properties of non-interacting (or quasi-free) fermions on the lattice. In particular, we recall some results obtained by J.B. Bru and W. de Siqueira Pedra few years ago on charge transport properties of systems of interacting fermions on lattices. By the end of the chapter, we also give preliminary results on the heat transport properties of quasi-free fermions, which are aimed to be a first step in order to get a quantum derivation of the well-known (classical) heat equation. The corresponding proofs are postponed to Chapter 7.
In Chapter 5, we give the most important results obtained during the thesis that are, Theorem 5.2.1 and Corollary 5.2.3, proven for non-interacting fermions but within a very general disordered media. They have been published in 2019, see [88]. We prove that the quantum uncertainty of microscopic electric current density around their classical values decreases exponentially fast with respect to the volume of the region where one applies an electric field. This is in accordance with the experiments made by B. Weber et al. in 2012, see [58]. This is an extension of the results of J.B. Bru and W. de Siqueira Pedra, see for instance [34] . Moreover, we propose some extension of the results that have been obtained in [88]. Actually, we give some estimation of the rate function that leads to the fast convergence of the quantum electrical currents towards their classical values. We prove in Theorem 5.4.1 that this is related to quantum fluctuations. This last result in not published yet, since it has been obtained lately within the pre-doctoral period, but should be used to write an additional paper in a near future.

Within Chapter 6, we prove that, in the semiclassical limit, the (classical) KMS condition can be derived from the quantum condition in the simple case of the Bose-Hubbard dynamical system on a finite graph, see Theorem 6.4.1 and Proposition 6.5.1. This work has been done in collaboration with Z. Ammari, based on a three months visit within the *Institut de Recherche Mathématiques de Rennes* in autumn 2018. This refers to the preprint [89], which has already been submitted.
Chapter 7 collects all technical proofs of the results of this thesis on charged and heat transport properties of non-interacting (or quasi-free) fermions on lattices. Finally, Chapter 8 is an appendix on the additional results that are important in the comprehension of this thesis. Essentially, this contains some standard theorems of functional analysis (semigroup theory) and also the mathematical foundations of the algebraic formulation of quantum mechanics. Note that the section on semigroup theory has been used to write a review article for graduate students and submitted to TEMat, a spanish journal that publishes informative works of mathematical students.

Resumen

Esta tesis es un estudio de las propiedades dinámicas y de equilibrio de los problemas cuánticos macroscópicos de muchos cuerpos. Una parte importante del manuscrito hace referencia al estudio de las propiedades de transporte de carga y calor de los fermiones en la red. Esto hace referencia a la derivación, a partir de los primeros principios de la mecánica y la termodinámica cuánticas, de la ley de Ohm -publicada por primera vez en 1827 por *G.S. Ohm* [1]-, y de la ecuación del calor -la conocida ecuación (clásica) establecida por *J. Fourier* en 1807 [2]-. Aún no se ha conseguido derivar por completo la ecuación del calor a partir de la mecánica cuántica, pero aquí demostramos algunos resultados preliminares relacionados con este tema no trivial. En cambio, en esta tesis se desarrolla en gran medida el estudio de las propiedades de transporte de carga de los sistemas de fermiones en la red. Esta es una cuestión fundamental en física, ya que, en la historia reciente, la creciente demanda de componentes electrónicos más pequeños ha aumentado el interés en el estudio de la teoría de la conductividad a escala atómica. La clásica ley de la conductividad de los materiales es la ley de Ohm. Es una observación empírica que afirma que el voltaje en un material conductor es directamente proporcional a la corriente que fluye a través de él, y que el coeficiente lineal correspondiente, es decir, la resistencia, crece proporcionalmente con respecto a la longitud de la muestra conductora. Se esperaba que esta teoría clásica de la conductividad de los materiales, basada en la existencia de una resistividad masiva bien definida, se degradase a medida que se alcanzan escalas atómicas y bajas temperaturas, ya que dominarían los efectos cuánticos. En concreto, la dependencia lineal de la resistencia en función de la longitud de los nanohilos conductores debería alterarse en las longitudes atómicas, como se explica en [42]. Sin embargo, en 2006, se verificó de manera experimental la validez de la teoría clásica, a temperatura ambiente, en nanohilos de arseniuro de indio (InAs) con longitudes de hasta 200nm [60]. De hecho, la resistividad medida en los nanohilos es de 23Ω/nm, que se aproxima mucho a la resistividad deducida a partir de las propiedades masivas del material (24Ω/nm). Véase [60, debate después de Ec. (2)]. Unos años más tarde, en 2012, se observó la misma propiedad [58], incluso a muy baja temperatura (4.2K) y longitudes de hasta 20 nm (escala atómica), en experimentos con nanohilos de silicio dopados con átomos de fósforo. Se espera [42] que la degradación de la descripción clásica de estos nanohilos esté alrededor de 10 nm (a una temperatura similar), ya que otros estudios experimentales [3, 4] en cables de silicio dopados similares muestran fuertes desviaciones respecto a los valores masivos de la resistividad alrededor de esta escala de longitud. Estos resultados experimentales demuestran que los efectos cuánticos sobre el transporte de cargas pueden desaparecer con suma rapidez con respecto a escalas espaciales crecientes. Este hecho lo demostramos matemáticamente al estudiar la tasa de supresión de la probabilidad de encontrar densidades de corriente microscópicas que difieran de la macroscópica, para fermiones en red sin interacción en un medio desordenado en equilibrio. Obsérvese que [34] ya ha probado la convergencia de los valores esperados de las densidades de corriente microscópicas, pero en el límite macroscópico no se obtuvo ninguna información acerca de

la supresión de la incertidumbre cuántica. Existen numerosas publicaciones matemáticas sobre las propiedades de transporte de carga de los fermiones en medios desordenados, como las de Bellissard y Schulz-Baldes en los años noventa [8, 9] o, más recientemente, las de Klein, Müller y otros [10, 13, 11, 12, 14]. Véase también [15, 16] y las referencias correspondientes, etc. Para una perspectiva histórica (no exhaustiva) de la conductividad lineal (Ley de Ohm), véase p. ej., [17], así como [33, 34, 32, 30, 29]. A pesar de todas esas publicaciones matemáticas sobre el transporte con carga cuántica, el estudio que se presenta en esta tesis abarca un aspecto teórico completamente nuevo de este problema, que aún no ha sido explotado en la bibliografía disponible. Este ha sido presentado recientemente, véase [88]. Similar a [34], buena parte de esta tesis está dedicada al caso no interactivo, pero el desorden es muy general, ya que se define a través de potenciales aleatorios y amplitudes aleatorias, complejas y saltantes, cuyas distribuciones ergódicas son solo una suposición. El célebre modelo Anderson de aproximación de enlace fuerte es un ejemplo particular del caso general analizado aquí y los modelos con potenciales vectoriales aleatorios también se incluyen en el presente estudio. En esta tesis, probamos, entre otras cosas, que la incertidumbre cuántica de las densidades de corriente eléctrica microscópica (alrededor de sus valores clásicos, macroscópicos) se suprime, de manera *exponencialmente rápida* con respecto al volumen $|\Lambda_L| = \mathcal{O}(L^d)$ (en unidades de la red, siendo la dimensión espacial $d \in \mathbb{N}$) de la región de la red donde se aplica un campo eléctrico externo. Para ello, se utiliza el formalismo de la gran desviación [38, 39], adoptado en la mecánica cuántica estadística desde los años ochenta [18, Sección 7]. Otros resultados matemáticos que son cruciales en nuestro análisis son las estimaciones de Combes-Thomas [36, 23], el teorema ergódico de Akcoglu-Krengel [37] y el teorema de Arzelà-Ascoli [54, Teorema A5]. En efecto, si se combina con el célebre teorema de Gärtner-Ellis (Teorema 5.1.1), nos permite probar el principio de grandes desviaciones (LDP, siglas en inglés de Large Deviation Principle) para las distribuciones de densidad de corriente, que cuantifica la probabilidad de desviación, debido a la incertidumbre cuántica, a partir del valor esperado. Además, proponemos una extensión de este último resultado. De hecho, ofrecemos una estimación de la tasa de cambio que lleva a la rápida convergencia de las corrientes eléctricas cuánticas hacia sus valores clásicos. En el Teorema 5.4.1 demostramos que está relacionado con las fluctuaciones cuánticas, que pueden considerarse como una variación desde el punto de vista de la teoría de la probabilidad. Este último resultado todavía no ha sido publicado, ya que se ha obtenido recientemente dentro del periodo predoctoral, pero debería usarse para escribir otro artículo en un futuro próximo. El caso de la interacción, como se estudia en [30, 29], tiene mayor relevancia a nivel técnico. Las técnicas mateméticas que permiten abordar estas cuestiones con los fermiones interactivos se han desarrollado parcialmente en [18, 19], y usan integrales de Grassmann y expansiones de la fórmula árbol de Brydges-Kennedy para la construcción de funciones generatrices de Gärtner-Ellis. Para el caso no-interactivo, con el fin de estudiar las propiedades de las funciones generatrices de Gärtner-Ellis, se puede utilizar la Desigualdad de Bogoliubov

$$\left|\ln \mathrm{tr}\left(C\mathrm{e}^{H_1}\right) - \ln \mathrm{tr}\left(C\mathrm{e}^{H_0}\right)\right| \leq \sup_{\alpha\in[0,1]} \sup_{u\in[-1/2,1/2]} \left\|\mathrm{e}^{u(\alpha H_1+(1-\alpha)H_0)}\left(H_1 - H_0\right)\mathrm{e}^{-u(\alpha H_1+(1-\alpha)H_0)}\right\|_{\mathcal{B}(\mathbb{C}^n)},$$

en la que H_0, H_1 son matrices arbitrarias autoadjuntas, C es cualquier matriz positiva y tr indica el trazo normalizado. Véase el Lema 7.2.3 má abajo. Lo anterior resulta útil para los sistemas fermiónicos casi libres (p. ej. H_0, H_1 son polinomios de grado dos en la creación fermiónica y operadores de aniquilación). En este caso especial, el lado derecho de la desigualdad está eficientemente delimitado por $\|H_1 - H_0\|_{\mathcal{B}(\mathbb{C}^n)}$, usando estimaciones de Combes-Thomas. Por el contrario, en el caso de los fermiones interactivos, se conocen ejemplos explícitos en los que el lado derecho es arbitrariamente mayor que $\|H_1 - H_0\|_{\mathcal{B}(\mathbb{C}^n)}$ en grandes volúmenes [24].

Nuestros resultados principales en cuanto a las propiedades de transporte de carga de fermiones no interactivos de la red son el Teorema 5.2.1, el Corolario 5.2.3 y el Teorema 5.4.1. Desde el punto de vista técnico, el Teorema 5.2.1 es una de las afirmaciones más importantes de esta tesis. Muchas otras afirmaciones, en particular el Principio de las Grandes Desviaciones para corrientes con una buena tasa de cambio (Teorema 5.2.2 y Corolario 5.2.3), se deducen del Teorema 5.2.1 a través de métodos estándar de grandes desviaciones. El Teorema 5.2.1 se refiere a la existencia, continuidad y diferenciación (volumen infinito) de la función determinista generadora de corrientes, que aparece en el teorema de Gärtner-Ellis (Teorema 5.1.1). Además de la Desigualdad de Bogoliubov, como se ha analizado anteriormente, su prueba necesita el teorema ergódico de Akcoglu-Krengel [37] como argumento importante, ya que ha de controlarse el límite termodinámico de las funciones generatrices (volumen finito) aleatorias. Para hacer posible el uso de este importante resultado de la teoría ergódica, se necesitan varios preliminares técnicos y la evidencia del Teorema 5.1.1 es altamente no trivial, en conjunto: Realizamos un desglose en caja bastante complicado de estas funciones aleatorias, que puede justificarse con la ayuda de la Desigualdad de Bogoliubov y con la localidad (descomposición espacial) tanto de la dinámica casi libre como de las correlaciones espaciales de los estados KMS, como consecuencia de las estimaciones de Combes-Thomas. A través de otros cálculos, el método anterior se ha ampliado posteriormente para estudiar más propiedades de regularidad de la función generatriz determinista (volumen infinito) de las corrientes. Esta extensión nos permite relacionar directamente la tasa funcional con las fluctuaciones cuánticas de las corrientes. Mientras tanto, en esta tesis se explica que estas fluctuaciones cuánticas generalmente no desaparecen, debido a la diferencia de la variable aleatoria, que define el medio desordenado. En conjunto, esto aporta una descripción bastante completa de las propiedades de transporte de carga de los fermiones no interactivos en la red.

Nótese que los estados de equilibrio en los que se estudian las propiedades de transporte de los fermiones libres se refieren a los estados KMS, una noción elegante del equilibrio introducida por *R. Kubo, P.C. Martin* y *J. Schwinger* a finales de los años cincuenta. Estos estados KMS, por supuesto, no se definen solamente para los sistemas de fermiones, sino para los sistemas generales. Son productos de la Segunda Ley de la Termodinámica, tal y como lo demostraron en 1978 *W. Pusz y S.L. Woronowicz* en [52]. Así que, además del estudio de las propiedades dinámicas de los sistemas de fermiones que se encuentran en un estado KMS inicial, en esta tesis también estudiamos la consecuencia de la condición KMS (cuántica) para un sistema de muchos *bosones* en la red en el límite semiclásico. Demostramos que la condición KMS clásica puede derivarse de la KMS (cuántica) para el sistema dinámico Bose-Hubbard en un grafo finito. Para llegar a ese resultado, consideramos un $\mathcal{W}^*$-sistema dinámico $(\mathcal{A}, \tau_t)$ que es un par de un álgebra de observables de von Neumann $\mathcal{A}$ y un grupo de un parámetro de automorfismos τ_t en $\mathcal{A}$. Considérese, por ejemplo, un espacio Hilbert de dimensiones finitas $\mathfrak{H}$, entonces $\mathcal{A}$ se puede elegir para ser el conjunto de todos los operadores $\mathcal{B}(\mathfrak{H})$ y τ_t como el grupo de automorfismo definido por

$$\tau_t(A) = e^{itH} A \, e^{-itH}$$

para cualquier $A \in \mathcal{A}$. El operador H representa el Hamiltoniano de un sistema cuántico determinado y el par $(\mathcal{A}, \tau_t)$ describe las dinámicas. Según la física estadística cuántica, este sistema admite un estado de equilibrio térmico único ω_β a temperatura inversa β dado por

$$\omega_\beta(A) = \frac{\mathrm{tr}(e^{-\beta H} A)}{\mathrm{tr}(e^{-\beta H})} \,. \tag{1}$$

En general, la sencillez de la afirmación anterior debe matizarse. De hecho, la caracterización del equilibrio térmico en la mecánica estadística es una cuestión no trivial, particularmente para los sistemas dinámicos que tienen un número infinito de grados de libertad, véase [27, 86]. Una de las caracterizaciones más importantes y elegantes de los estados de equilibrio fue observada por R. Kubo, P.C. Martin y J. Schwinger a finales de los años cincuenta. Se basa en las siguientes observaciones en una dimensión finita. De hecho, se observa a través de un simple cálculo que el estado de Gibbs ω_β en (1) cumple para todos los $t \in \mathbb{R}$ y cualquier $A, B \in \mathcal{A}$ la identidad

$$\omega_\beta(A \; \tau_{t+i\beta}(B)) = \omega_\beta(\tau_t(B) A) \tag{2}$$

donde $\tau_{t+i\beta}(\cdot)$ indica una extensión analítica del automorfismo τ_t para tiempos complejos dados por

$$\tau_{t+i\beta}(B) = e^{(-\beta+it)H} B \, e^{(\beta-it)H} \,.$$

Más notable, si se toma un estado ω que satisface la misma condición que (2), entonces ω debería ser el estado de Gibbs ω_β en (1). Esto indica que la ecuación (2) señala los estados de equilibrio térmico entre todos los estados posibles de un sistema cuántico. A finales de los años sesenta, R. Haag, N.M. Hugenholtz y M. Winnink sugirieron la identidad (2) como un criterio para los estados de equilibrio y la denominaron condición límite KMS en honor a Kubo, Martin y Schwinger [79]. El tema de los estados KMS se está estudiando en profundidad, especialmente desde un punto de vista algebraico. Por ejemplo, se han derivado varias caracterizaciones relacionadas con las desigualdades de correlación y con los principios variacionales (véase, p. ej. [73, 68]). También se han explorado otras perspectivas relacionadas, por ejemplo, con la teoría de Tomita-Takasaki y con el álgebra de Heck y la teoría de números (véase, p. ej. [71, 67, 69]).

En los años setenta, G. Gallavotti y E. Verboven sugirieron una analogía de la condiciín límite KMS (2), que sirve para los sistemas mecánicos clásicos y destacaron su relación con las ecuaciones de Kirkwood-Salzburg y con las medidas de equilibrio de Gibbs, véase [78].

La derivación de esta condición se basa en el siguiente argumento heurístico. Considérese un estado que $\omega_\hbar$ satisface la condición límite KMS

$$\omega_\hbar\Big(BA\Big) = \omega_\hbar\Big(A\,\tau_{i\hbar\beta}(B)\Big) \tag{3}$$

a temperatura inversa $\hbar\beta$, donde $\hbar$ se refiere a la constante de Planck reducida. Esta relación produce

$$\omega_\hbar\Big(\frac{AB-BA}{i\hbar}\Big) = \omega_\hbar\Big(A\;\frac{\tau_{i\hbar\beta}(B)-B}{i\hbar}\Big).$$

Supongamos por un momento que el espacio $\mathfrak{H} = L^2(\mathbb{R}^d)$ por lo que se puede considerar que el Hamiltoniano H y las observables A, B vienen dadas por los símbolos cuantizados $\hbar$-Weyl (p. ej. $H = h^{W,\hbar}$, $A = a^{W,\hbar}$, y $B = b^{W,\hbar}$ para algunas funciones lisas a y b definidas sobre el espacio de fase $\mathbb{R}^{2d}$). Entonces la teoría semiclásica nos dice primero que

$$\frac{AB-BA}{i\hbar} \underset{\hbar\to 0}{\longrightarrow} \{a,b\}\,, \qquad \text{y} \qquad \frac{\tau_{i\hbar\beta}(B)-B}{i\hbar} \underset{\hbar\to 0}{\longrightarrow} \beta\,\{h,b\}\,, \tag{4}$$

donde $\{\cdot,\cdot\}$ es el corchete de Poisson y h denota el Hamiltoniano del sistema clásico correspondiente. En segundo lugar, los estados cuánticos $\omega_\hbar$ (o, al menos, una subsucesión) convergen en un sentido débil a una medida de probabilidad semiclásica μ sobre $\mathbb{R}^{2d}$ cuando $\hbar \to 0$. Por lo tanto, la condición clásica esperada de KMS que en principio debería caracterizar el equilibrio estadístico de los sistemas mecánicos clásicos viene dada formalmente por

$$\mu\Big(\{a,b\}\Big) = \beta\,\mu\Big(a\,\{h,b\}\Big)\,, \tag{5}$$

para cualquier función lisa a, b en el espacio de fase $\mathbb{R}^{2d}$. Aquí se usa la notación $\mu(f) = \int_{\mathbb{R}^{2d}} f(u)\,d\mu(u)$. Después de los trabajos [78, 63], M. Aizenman et al. mostraron en [64] que la condición (5) se*ñ*ala estados de equilibrio térmico para sistemas mecánicos clásicos infinitos entre todas las medidas de probabilidad. En particular, la única medida μ que satisface (5) en nuestro ejemplo es la medida de Gibbs definida con respecto a la medida de Lebesgue por la densidad,

$$\mu_\beta = \frac{1}{z(\beta)}\; e^{-\beta h(u)}\,, \tag{6}$$

donde $z(\beta)$ es una constante de normalización. Nótese que la medida de Gibbs anterior μ_β también puede ser caracterizada como un estado de equilibrio por medio de métodos variacionales y propiedades de máxima entropía o por desigualdades de correlación, véase [27]. Sin embargo, en esta tesis nos centramos solo en las condiciones límite KMS para sistemas clásicos y cuánticos. En general, la derivación de la condición límite KMS clísica (5) a partir de la cuántica es una cuestión no trivial e interesante que depende del sistema dinámico considerado. En nuestra opinión, la condición KMS clásica es una caracterización elegante del equilibrio estadístico que merece más atención por parte de los analistas de PDE. Aunque esta condición ha sido estudiada en algunos trabajos posteriores (véase p. ej. [77, 83, 85, 84, 70, 74]), no es muy conocida.

En esta tesis, proporcionamos una prueba rigurosa y sencilla de la derivación de la condición KMS clásica (5) como consecuencia de la relación (2) y el límite clásico $\hbar \to 0$ para el sistema dinámico de Bose-Hubbard en un grafo finito. El sistema que consideramos que está gobernado por un típico Hamiltoniano cuántico de muchos cuerpos que puede ser escrito en términos de operadores de aniquilaciones de creaciones y que está restringido a un volumen finito. Nuestra prueba de convergencia se basa en la Desigualdad de Golden-Thompson, la Desigualdad de Bogoliubov y el análisis semiclásico en el espacio de Fock. Dado que el espacio de fase clásico del sistema que se considera aquí es de dimensiones finitas, es posible, mediante un cambio de representación, convertir el problema en un análisis semiclásico en un espacio L^2. Sin embargo, evitamos ese cambio ya que perdemos la mayor parte de la perspectiva y la mayoría de las estructuras interesantes de nuestro problema. En particular, nos basaremos en el análisis del espacio de fase que figura en [65]. Nuestro interés en el sistema de Bose-Hubbard está motivado por el establecimiento de un fuerte vínculo entre las condiciones KMS clásicas y cuánticas, de modo que conduce al intercambio de los límites termodinámicos y clásicos por sistemas dinámicos infinitos y a la investigación de las transiciones de fase. Nótese también que, desde un punto de vista físico, el modelo de Bose-Hubbard es un modelo bastante relevante que describe átomos extremadamente fríos en redes ópticas con un fenómeno observado de transición superfluido-aislante. Desde una perspectiva más amplia, la pregunta que se considera aquí también está relacionada con la tendencia reciente iniciada por M. Lewin, P.T. Nam y N. Rougerie [81, 82] sobre las medidas de Gibbs para las ecuaciones no lineales de Schrödinger (véase también [76] donde continuaron estas investigaciones). En este sentido, las condiciones límite KMS podrían constituir una prueba alternativa de la convergencia de los estados de Gibbs. Estas cuestiones serán consideradas en otro lugar y, como estudio preliminar, en esta tesis solo nos centraremos en el modelo de Bose-Hubbard en un grafo finito, que es un modelo mucho más sencillo.

Plan de trabajo

El capítulo 1 tiene como objetivo plantear al lector las primeras intuiciones acerca de la formulación mecánica cuántica. En particular, introducimos la formulación algebraica de la mecánica cuántica, en la que la estructura de espacio de Hilbert ya no es el eje de la estructura. Sin embargo, recordamos el vínculo entre la formulación algebraica y la formulación basada en un espacio de Hilbert al final del capítulo.
En el capítulo 2, explicamos el conocido concepto del estado de equilibrio, que es fundamental en esta tesis. De hecho, todos los sistemas que se consideran aquí se encuentran en estado de equilibrio. Para definir el estado de equilibrio, se puede, por ejemplo, utilizar un problema variacional correspondiente para minimizar la entropía de la energía libre. Aquí nos apoyamos en la noción del estado KMS, que está relacionada con la Segunda Ley de la Termodinámica y la llamada pasividad completa de un estado de equilibrio. La Segunda Ley tiene su origen en la obra de N.L.S. Carnot del siglo XIX, y todavía hoy se utiliza a través de obras matemáticas de E.H. Lieb, J. Yngvason y otros investigadores como W. Pusz, S.L. Woronowicz, J.B. Bru y W. de Siqueira Pedra.
En el capítulo 3, presentamos la formulación algebraica de los problemas cuánticos de muchos cuerpos. Un marco estándar para entender esta construcción es el conocido espacio de Fock, que será explicado por razones pedagógicas. Debido a la distinción entre fermiones y bosones, desarrollamos las dos formas de formulación algebraica de problemas cuánticos de muchos cuerpos.
En el capítulo 4 recoge las herramientas que se han usado directamente para formular correctamente los resultados que obtuvimos durante la tesis sobre las propiedades de transporte de los fermiones. En particular, recordamos algunos de los resultados obtenidos por J.B. Bru y W. de Siqueira Pedra hace unos años sobre las propiedades de transporte de carga. Al final del capítulo, también damos resultados preliminares sobre las propiedades de transporte, que pretenden ser un primer paso para obtener una derivación cuántica de la conocida ecuación (clásica) del calor. Las pruebas correspondientes se dejan para el capítulo 7.
En el capítulo 5, damos los resultados más importantes obtenidos durante la tesis, que son el Teorema 5.2.1 y el Corolario 5.2.3. Han sido publicados en 2019, véase [88]. Demostramos que la incertidumbre cuántica de la densidad de corriente eléctrica microscópica alrededor de sus valores clásicos disminuye exponencialmente rápido respecto al volumen de la región donde se aplica un campo eléctrico. Esto se ajusta a los experimentos realizados por B. Weber et al. en 2012, véase [58]. Esta es una extensión de los resultados de J.B. Bru y W. de Siqueira, véase por ejemplo [34]. Además, proponemos una cierta extensión de los resultados que han sido obtenidos en [88]. De hecho, ofrecemos una estimación de la función de la tasa de cambio que lleva a la rápida convergencia de las corrientes eléctricas cuánticas hacia sus valores clásicos. En el Teorema 5.4.1 demostramos que esto está relacionado con las fluctuaciones cuánticas. Este último resultado aún no ha sido publicado, ya que se ha obtenido recientemente, dentro del periodo predoctoral, pero debería usarse para escribir otro artículo en un futuro próximo.

En el capítulo 6, demostramos que, en el límite semiclásico, la condición (clásica) KMS puede derivarse de la condición cuántica en el caso sencillo del sistema dinámico de Bose-Hubbard en un grafo finito, véase el Teorema 6.4.1 y la Propuesta 6.5.1. Este trabajo se ha realizado en colaboración con Z. Ammari, a partir de una visita de tres meses al Institut de Recherche Mathématiques de Rennes en otoño del 2018. Esto se refiere a la preimpresión [89], la cual ya ha sido presentada para su publicación.
El capítulo 7 recoge todas las pruebas técnicas de los resultados de esta tesis sobre las propiedades de transporte de carga y de calor. Finalmente, el capítulo 8 es un apéndice sobre los resultados adicionales que son relevantes para la comprensión de esta tesis. Básicamente, contiene algunos teoremas estándar de análisis funcional (teoría de semigrupos) y también las bases matemáticas de la formulación algebraica de la mecánica cuántica. Nótese que la sección de teoría de semigrupos se ha usado para escribir un trabajo de revisión para estudiantes de posgrado y se ha enviado a TEMat, una revista española que publica trabajos informativos de estudiantes de matemáticas.

Notation

- We denote by $D \in \mathbb{R}_0^+$ a generic constant. These constants do not need to be the same from one statement to another.
- The norm on a generic vector space $\mathcal{X}$ is denoted by $\|\cdot\|_{\mathcal{X}}$.
- The identity element of a generic vector space $\mathcal{X}$ is denoted by $\mathbf{1}_{\mathcal{X}}$.
- The set of linear operators from $\mathcal{X}$ into itself is denoted by $\mathcal{L}(\mathcal{X})$.
- The Banach space of all bounded linear operators on $(\mathcal{X}, \|\cdot\|_{\mathcal{X}})$ is denoted by $\mathcal{B}(\mathcal{X})$. For an operator $A \in \mathcal{B}(\mathcal{X})$, its norm is defined by

$$\|A\|_{\mathcal{B}(\mathcal{X})} := \sup_{u \in \mathcal{X} \setminus \{0\}} \frac{\|Au\|_{\mathcal{X}}}{\|u\|_{\mathcal{X}}}.$$

- If $\mathcal{X}$ is a Hilbert space then its norm is associated to a scalar product denoted by $\langle \cdot, \cdot \rangle_{\mathcal{X}}$.
- For all $A, B \in \mathcal{B}(\mathcal{X})$, we define

$$[A, B] := AB - BA \quad \text{and} \quad \{A, B\} := AB + BA.$$

- For any complex number z, its conjugate is denoted by $\bar{z}$.
- $\mathbb{K}[X]$ denotes the set of polynomials with coefficients in the ring $\mathbb{K}$.

Contents

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Chapter 1

Introduction

1.1 Introduction

In the mid-20's, two main formulations of quantum physics appeared, both were meant to establish the principles of quantum theory. These two directions were taken for one side by W.K. Heisenberg and for the other one by E. Schrödinger. After being in opposition, they appeared to be equivalent after several contributions of J. von Neumann on the foundation of quantum mechanics in the following years. Both approaches are currently used in any standard text book on quantum physics. For the sake of clarity, we will first set the so-called *Schrödinger picture* of quantum mechanics. Indeed, despite the fact that in the context of this thesis, we are following the path led by W.K. Heisenberg, the *Schrödinger picture* seems to be more useful for the intuition of any reader, being widely known, used and commented such as in the field of Partial Differential Equations (PDEs), for instance, through the celebrated *Schrödinger equation*.

Schrödinger Picture of quantum mechanics

In 1925, following de Broglie's hypothesis on wave property of matter, E. Schrödinger derived his celebrated equation, describing a time-dependent wave behavior of quantum objects. In fact, the state of the quantum system is completely described by a family of time dependent wave functions $\{\psi(t)\}_{t\in\mathbb{R}}$ within a Hilbert space $\mathcal{H}$. For instance, one generally considers the case $\mathcal{H} := L^2(\mathbb{R}^3)$ or $\mathcal{H} := \ell^2(\mathbb{Z}^3)$, respectively for the continuum quantum system or the discrete one. This time evolution is fixed by a self-adjoint operator H acting on $\mathcal{H}$. Indeed, for any time $t \in \mathbb{R}$, the wave function is determined by the well-known *Schrödinger equation*:

$$(SE)\begin{cases} i\partial_t\psi(t) = H\psi(t). \\ \psi(0) = \psi_0 \in \mathcal{H}. \\ = \end{cases} \tag{1.1}$$

This implies that

$$\psi(t) = \mathrm{e}^{-itH}\psi_0, \quad t \in \mathbb{R}. \tag{1.2}$$

Note that the fact that H is self adjoint is important to give a sense to Equations (1.1)-(1.2). It is described through Stone's theorem [53, VIII.4], which sets that having a self-adjoint operator, acting on some Hilbert space, is a sufficient condition in order to define a strongly continuous one-parameter group. We will say some words on them later but, at this point, the aim is to give an intuition to the reader about the different ways to formulate quantum mechanics. A standard example taught to every student in quantum mechanics is brought by the case where $\mathcal{H} := L^2(\mathbb{R}^3)$ and $\|\psi(t)\|_{\mathcal{H}} = \|\psi_0\|_{\mathcal{H}} = 1$. Then $|\psi(t,x)|^2$ is interpreted as the probability for the particle to be at a position $x \in \mathbb{R}^3$ at time $t \in \mathbb{R}$. The same interpretation can be done on the lattice $\mathbb{Z}^3$, instead of taking $\mathbb{R}^3$.

Heisenberg Picture of quantum mechanics

Physical quantities such as position, speed, energy, etc... are self adjoint operators acting on $\mathcal{H}$. They are called *observables*, being all quantities of the physical system that can be measured. For instance, one of the most important *observable* is the celebrated self adjoint *Hamiltonian* H that describes the time evolution of wave function in the *Schrodinger Equation* (1.1)-(1.2). This *Hamiltonian* is associated with the energy *observable*.

The measurement of a physical quantity (*observable*) has, in this point of view, a random character. The statistical distribution of its value is described by the family of wave functions $\{\psi(t)\}_{t\in\mathbb{R}}$ (see Equation (1.1)).The expectation value of any *observable* B acting on $\mathcal{H}$ is given by

$$\langle \psi(t), B\psi(t)\rangle_{\mathcal{H}} . \tag{1.3}$$

By Equation (1.2), it equals

$$\langle \psi(t), B\psi(t)\rangle_{\mathcal{H}} = \left\langle \psi_0, \mathrm{e}^{itH} B \mathrm{e}^{-itH} \psi_0 \right\rangle_{\mathcal{H}} . \tag{1.4}$$

At this point, it turns out that, instead of considering the wave functions as being time-dependent, like in Schrödinger Picture of quantum mechanics, one can take them as fixed in time and assume a time evolution of the so-called *observables*. Both methods lead to the same statistical distribution as one can see in Equation (1.4). Indeed, for the time evolution of any *observable* B, we apply on it the map $\tau_t(B) := \mathrm{e}^{itH} B \mathrm{e}^{-itH}$ for $t \in \mathbb{R}$. For any $H \in \mathcal{B}(\mathcal{H})$, the family $\{\tau_t\}_{t\in\mathbb{R}}$ defines a continuous group acting on the Banach space $\mathcal{B}(\mathcal{H})$ of all bounded linear operators on $\mathcal{H}$ and satisfies the following evolution equation, for all $t \in \mathbb{R}$:

$$\partial_t \tau_t = \tau_t \circ \delta = \delta \circ \tau_t, \quad \tau_0 = \mathbf{1}_{\mathcal{X}}, \tag{1.5}$$

where the generator δ is defined by

$$\delta(B) := i\,[H, B]\,, \quad B \in \mathcal{B}(\mathcal{H}). \tag{1.6}$$

Note that $\{\tau_t\}_{t\in\mathbb{R}}$ is a family of isomorphisms of $\mathcal{B}(\mathcal{H})$ and, for all $A, B \in \mathcal{B}(\mathcal{H})$, one has

$$\delta(A^*) = \delta(A)^* \quad \text{and} \quad \delta(AB) = \delta(A)B + A\delta(B). \tag{1.7}$$

An operator satisfying (1.7) is called a *symmetric derivation* or $*$*-derivation*. Note that $A^* \in \mathcal{B}(\mathcal{H})$ is the usual adjoint operator of $A \in \mathcal{B}(\mathcal{H})$. Once again, more precise definitions of the mathematical tools that are involved to formulate quantum problems will be given later, since it is not necessary at this point. Indeed, for the moment, the aim is to give an intuition to the reader about the different mathematical approaches that can be taken to describe quantum systems.

1.2 Algebraic quantum mechanics

C^*-dynamical system for quantum mechanics

Instead of beginning with the Schrödinger equation and fixing a Hilbert space as a fundamental starting point to formulate quantum problems, the algebraic quantum mechanics takes the Heisenberg picture of quantum mechanics as a starting point. Indeed, one uses a pair $(\mathcal{X}, \tau)$ which is usually called C^*-dynamical system. The first component is a C^*-algebra while the second one is a family of $*$-automorphisms acting on $\mathcal{X}$. This approach generalizes the concept of *observables* as operators acting on a Hilbert space $\mathcal{H}$, and the time evolution briefly introduced above. To understand this, we first say some words about C^*-algebras and $*$-automorphisms.

C^*-Algebra for quantum mechanics

Let $\mathcal{X} := (\mathcal{X}, +, \cdot)$ be a $\mathbb{C}$-vector space with a natural product for any $A, B \in \mathcal{X}$, $A \cdot B := AB$. Assume moreover that $\mathcal{X}$ is an associative, distributive and unital algebra. Unital algebra refers to the fact that there exists an element $\mathbf{1} \in \mathcal{X}$ such that $A \cdot \mathbf{1} = \mathbf{1} \cdot A = A$ for all $A \in \mathcal{X}$. From this, to introduce the notion of C^*-algebra, we need first to define the concept of antilinear involution:

Definition 1.2.1 (Antilinear involution and $*$-algebra)
An antilinear involution of an algebra $\mathcal{X}$ is a map:

$$\mathcal{X} \to \mathcal{X}, \quad A \mapsto A^*$$

that satisfies

i) for all $A \in \mathcal{X}$: $(A^*)^* = A$,

ii) for all $A, B \in \mathcal{X}$: $(AB)^* = B^* A^*$,

iii) for all $A, B \in \mathcal{X}$ and $a, b \in \mathbb{C}$: $(aA + bB)^* = \bar{a}A^* + \bar{b}B^*$.

$A^* \in \mathcal{X}$ is called the adjoint element of A. One says that $\mathcal{X} := (\mathcal{X}, +, \cdot, *)$ is a $*$-algebra.

Now let us provide a norm to our vector space and define $\mathcal{X} := (\mathcal{X}, +, \cdot, *, \|\cdot\|_{\mathcal{X}})$ as a Banach $*$-algebra with norm $\|\cdot\|_{\mathcal{X}}$. We are now in a position to give a definition of a C^*-algebra:

Definition 1.2.2 (C^*-algebra)
A Banach $*$-algebra $\mathcal{X} := (\mathcal{X}, +, \cdot, *, \|\cdot\|_{\mathcal{X}})$ such that, for all $A \in \mathcal{X}$, $\|A^* \cdot A\|_{\mathcal{X}} = \|A\|_{\mathcal{X}}^2$ is called a C^*-algebra.

Remark 1.2.3 (Equality of norms)
From properties of the norm in a Banach algebra and the definition of a C^*-algebra,

$$\|A\|_{\mathcal{X}}^2 = \|A^* \cdot A\|_{\mathcal{X}} \leq \|A^*\|_{\mathcal{X}} \|A\|_{\mathcal{X}}.$$

This holds true by switching A and A^* for any $A \in \mathcal{X}$. Therefore,

$$\|A\|_{\mathcal{X}} = \|A^*\|_{\mathcal{X}}.$$

Remark 1.2.4 (Unicity of the C^*-norm)
Given a $*$-algebra it is well-known that there is a unique norm turning the $*$-algebra into a C^*-algebra, see [25, Proposition 1-2].

Note that self-adjoint elements A of a C^*-algebra $\mathcal{X}$ are those satisfying $A = A^*$. They are called *observables*. This can be justified by the fact that their spectra are included in the set of real numbers. In terms of physics, it gives a sense to the *measurement of physical quantities*.

We introduce now a special case of C^*-algebra that will be useful latter: the von Neumann algebra. Recall that, when we introduce the Heisenberg Picture in section 1.1, we set that physical quantities are represented by self-adjoint operators acting on a Hilbert space $\mathcal{H}$. Therefore, for any operator $A \in \mathcal{B}(\mathcal{H})$, define the usual operator norm

$$\|A\|_{\mathcal{B}(\mathcal{H})} := \sup_{x \in \mathcal{H}, \|x\|_{\mathcal{H}} = 1} \|Ax\|_{\mathcal{H}} < \infty.$$

Then $(\mathcal{B}(\mathcal{H}), \|\cdot\|, \cdot, *)$ is a unital C^*-algebra. Again, note that the involution is obtained here by taking the adjoint operator.

For any Hilbert space $\mathcal{H}$ and any $\mathcal{M} \in \mathcal{B}(\mathcal{H})$, let $\mathcal{M}'$ denote its commutant, that is, the set of bounded operators on $\mathcal{H}$ commuting with each element of $\mathcal{M}$. For more details, see [26, Section 2.4.2] as well as [61] and [62]. Von Neumann algebras are particular $*$-subalgebra of $\mathcal{B}(\mathcal{H})$:

Definition 1.2.5 (von Neumann algebra)
Let $\mathcal{H}$ be an Hilbert space. A von Neumann algebra on $\mathcal{H}$ is a $*$-subalgebra of $\mathcal{B}(\mathcal{H})$ such that

$$\mathcal{M} = \mathcal{M}''.$$

Endowed with the operator norm, i.e., the norm of $\mathcal{B}(\mathcal{H})$, $\mathcal{M}$ is a C^*-algebra, by the bicommutant theorem [26, Theorem 2.4.11]. For more details about the theory of C^*-algebra, a reference book on the theory of C^*-algebra is [61]. See also [62] for a recent compendium on operator algebras. [26] is also a standard text book related to *Operator Algebras and Quantum Statistical Mechanics*. Now, as already mentioned above, we are going to describe the time evolution of those *observables*, which comes from a family of $*$-automorphisms.

$*$-Automorphism of C^*-algebra

For two unital C^*-algebras $\mathcal{X}$ and $\mathcal{Y}$, a linear map

$$\pi : \mathcal{X} \to \mathcal{Y}$$

is a $*$-homomorphism if, for all $a, b \in \mathbb{C}$ and $A, B \in \mathcal{X}$,

$$\pi(aA + bB) = a\pi(A) + b\pi(B), \quad \pi(AB) = \pi(A)\pi(B), \quad \text{and} \quad \pi(A^*) = \pi(A)^*. \tag{1.8}$$

Such a π is contractive and even isometric when it is injective, as stated in [26, Proposition 2.3.1 and Proposition 2.3.3]. Moreover, if π is bijective then it is called $*$-isomorphism. In particular, a $*$-isomorphism from $\mathcal{X}$ to itself is called a $*$-automorphism of $\mathcal{X}$. For $H \in \mathcal{B}(\mathcal{H})$, an example is given by the family $\{\tau_t\}_{t\in\mathbb{R}}$ defined by.

$$\tau_t(B) := \mathrm{e}^{itH} B \mathrm{e}^{-itH}, \quad B \in \mathcal{B}(\mathcal{H}),\ t \in \mathbb{R}. \tag{1.9}$$

Compare with Equation (1.4). A basic computation implies that, for each $t \in \mathbb{R}$, τ_t defines a $*$-automorphism. Using this pedagogical example, it is easy to compute its norm: By using the property of C^*-algebra, for $H \in \mathcal{B}(\mathcal{H})$, one has

$$\left\|\mathrm{e}^{itH}\right\|^2_{\mathcal{B}(\mathcal{H})} = \left\|\left(\mathrm{e}^{itH}\right)^* \mathrm{e}^{itH}\right\|_{\mathcal{B}(\mathcal{H})} = \left\|\mathrm{e}^{-itH}\mathrm{e}^{itH}\right\|_{\mathcal{B}(\mathcal{H})} = 1.$$

Therefore, for any $B \in \mathcal{B}(\mathcal{H})$, by using the norm property of a Banach space

$$\|\tau_t(B)\|_{\mathcal{B}(\mathcal{H})} \leq \left\|\mathrm{e}^{itH}\right\|_{\mathcal{B}(\mathcal{H})} \|B\|_{\mathcal{B}(\mathcal{H})} \left\|\mathrm{e}^{-itH}\right\|_{\mathcal{B}(\mathcal{H})} = \|B\|_{\mathcal{B}(\mathcal{H})}.$$

and, since $\tau_t(\mathbf{1}_{\mathcal{B}(\mathcal{H})}) = 1$, we deduce that

$$\|\tau_t\|_{\mathcal{B}(\mathcal{B}(\mathcal{H}))} := \sup_{B\in\mathcal{B}(\mathcal{H})\backslash\{0\}} \frac{\|\tau_t(B)\|_{\mathcal{B}(\mathcal{H})}}{\|B\|_{\mathcal{B}(\mathcal{H})}} = 1, \quad t \in \mathbb{R}. \tag{1.10}$$

This property is satisfied by any $*$-automorphism of a C^* -algebra. We are know able to detail the algebraic approach of quantum mechanics.

1.3 Algebraic formulation of quantum mechanics

Algebraic formulation of Heisenberg picture of quantum mechanics

A physical system is described by a non-empty set of all physical quantities that can be measured within this system. This non-empty set will be denoted here by $\mathcal{O}$ and is a set of self-adjoint elements of a unital C^*-algebra $\mathcal{X}$. An element of $\mathcal{O}$ is an *observable*. For any *observable*, its spectrum is a subset of $\mathbb{R}$ and represents all the values that can result from the measurement of the corresponding physical quantity. The quantum dynamics is given by a strongly continuous one-parameter group of $*$-automorphisms.

Definition 1.3.1 (Autonomous C^*-dynamical system)
Let $\mathcal{X}$ be a unital C^*-algebra. A family $\{T_t\}_{t\in\mathbb{R}}$ of automorphisms of $\mathcal{X}$ is a group of automorphisms if

1. $T_0 = 1_{\mathcal{X}}$,
2. $\forall t, s \in \mathbb{R} : \; T_{t+s} = T_t \circ T_s$.

Moreover, $(\mathcal{X}, \{T_t\}_{t\in\mathbb{R}})$ is an autonomous C^*-dynamical system if this group is strongly continuous, i.e., for all $B \in \mathcal{X}$, $t \mapsto T_t(B)$ is a continuous function from $\mathbb{R}$ to $\mathcal{X}$.

Definition 1.3.2 (Generator of C^*-dynamical system)
Let $(\mathcal{X}, \{T_t\}_{t\in\mathbb{R}})$ be an autonomous C^*-dynamical system. Define the linear subspace

$$\mathcal{D}(G) := \{A \in \mathcal{X} : t \mapsto T_t(A) \text{ is differentiable at } t = 0\}.$$

Define also the linear operator by $G : \mathcal{D}(G) \to \mathcal{X}$ by

$$G(A) := \frac{d}{dt} T_t(A)|_{t=0}.$$

G is called the generator of the C^*-dynamical system and $\mathcal{D}(G)$ is the domain of G. See Appendix 2 in Section 8.2 for more details on the existence of generators of strongly continuous semigroups. This Appendix is widely inspired by [41] on semigroup theory.

In the context of this work, the time evolution of our quantum system will be described by $\tau := \{\tau_t\}_{t\in\mathbb{R}}$, which is a family of strongly continuous group of $*$-automorphisms generated by a symmetric derivation δ acting on $\mathcal{X}$, see Equation (1.7). It satisfies the autonomous evolution equation defined, for $t \in \mathbb{R}$, by

$$\partial_t \tau_t = \tau_t \circ \delta = \delta \circ \tau_t, \quad \tau_0 = \mathbf{1}_{\mathcal{X}}.$$

Note that δ can be an unbounded operator acting on $\mathcal{X}$. Following Definition 1.3.1, the couple $(\mathcal{X}, \tau)$ is called a C^**-(autonomous) dynamical system*.

Algebraic formulation of Schrödinger picture of quantum mechanics

In section 1.1, when we started by giving some intuitions about the formulation of a quantum problem from the *Schrödinger equation*, we have seen that the state of our physical system is completely described by the family of time-dependent wave functions $\{\psi(t)\}_{t\in\mathbb{R}}$ within some Hilbert space $\mathcal{H}$. For any $B \in \mathcal{B}(\mathcal{H})$ (which can be seen as a C^*-algebra, see Section 1.2), Equation (1.3) describes a map:

$$B \mapsto \langle \psi(t), B\psi(t)\rangle_{\mathcal{H}},$$

which is a positive and normalized linear functional from $\mathcal{B}(\mathcal{H})$ to $\mathbb{C}$, as soon as the initial state is normalized, i.e., $\|\psi_0\|_{\mathcal{H}} = \|\psi(0)\|_{\mathcal{H}} = 1$. In the algebraic formulation, states on a C^*-algebra $\mathcal{X}$ are continuous linear functionals from $\mathcal{X}$ to $\mathbb{C}$, denoted by ρ, which are normalized and positive, i.e., satisfying

$$\rho(\mathbf{1}_{\mathcal{X}}) = 1 \quad \text{and} \quad \rho(B^*B) \geq 0, \quad \forall B \in \mathcal{X}.$$

Recall that $\mathbf{1}_{\mathcal{X}}$ is the identity element of $\mathcal{X}$. Those positive normalized linear functionals represent the state of physical systems and give the statistical distribution of the measures of any *observable* $B \in \mathcal{X}$. Note that if one takes a strongly continuous group $\{\tau_t\}_{t\in\mathbb{R}}$ of $*$-automorphisms of $\mathcal{X}$ then

$$\rho_t := \rho \circ \tau_t, \quad \forall t \in \mathbb{R}$$

is also a *state*. Then, in the Schrödinger Picture, the dynamics is given by the family of states $\left\{\rho_t\right\}_{t\in\mathbb{R}}$. Note that from [26, lemma 2.3.10], for any *state*, being by definition a positive functional, the following assertion holds true:

Lemma 1.3.3 (Cauchy-Schwarz inequality) .
Let $\mathcal{X}$ be a unital C^*-algebra and ρ a positive linear functional from $\mathcal{X}$ to $\mathbb{C}$. Then for $A, B \in \mathcal{X}$,

i) $\rho(A^*B) = \overline{\rho(B^*A)}$,

ii) $|\rho(A^*B)|^2 \leq \rho(A^*A)\rho(B^*B)$.

Proof: Let $\rho : \mathcal{X} \to \mathbb{C}$ be a positive linear functional. Observe that, for all $A, B \in \mathcal{X}$, one has

$$\rho\left((A + B)(A + B)^*\right) = \rho(A^*A) + \rho(A^*B) + \rho(B^*A) + \rho(B^*B) \geq 0.$$

It follows that, for all $A, B \in \mathcal{X}$,

$$\rho(A^*B) + \rho(B^*A) \in \mathbb{R}, \tag{1.11}$$

i.e., *i)* holds true. Now, from *i)*, one can define an inner product on $\mathcal{X}$ by

$$\langle A, B\rangle_\rho := \rho(A^*B), \qquad A, B \in \mathcal{X}.$$

Then, one obtains the second assertion by applying the *Cauchy-Schwarz inequality* on $\langle\cdot,\cdot\rangle_\rho$.
■

Remark 1.3.4 (Self-adjoint elements as *observables*)
For any $A \in \mathcal{X}$, taking $B = \mathbf{1}_{\mathcal{X}}$ in Lemma 1.3.3 yields to

$$\rho(A) = \overline{\rho(A^*)}.$$

Taking self-adjoint elements $A = A^* \in \mathcal{X}$ as observables gives then a sense to the "measurement" of a physical quantity since, in this case, the outcome $\rho(A)$ is a real number.

In the algebraic formulation of quantum mechanics, one does not need to fix a Hilbert space structure. Nevertheless, the celebrated *Gelfand-Naimark-Segal* (GNS) construction gives a relation between both, through a representation of C^*-algebra. This is explained in the next section.

1.4 Representation of C^*-algebra

In this part, we explain the relation between the algebraic formulation of quantum mechanics, starting from a C^*-algebra, and its Hilbert space formulation. Let $\mathcal{X}$ be a C^*-algebra. The pair $(\pi, \mathcal{H})$, where $\mathcal{H}$ is a Hilbert space and π a $*$-homomorphism from $\mathcal{X}$ to $\mathcal{B}(\mathcal{H})$, is called, in the literature, the representation of $\mathcal{X}$. This representation is faithful whenever π is injective. Moreover, if there exists an element A_0 of $\mathcal{H}$ such that

$$\overline{\pi(\mathcal{X})A_0} = \mathcal{H}$$

then A_0 is called a cyclic vector of $\mathcal{H}$. The triplet $(\pi, \mathcal{H}, A_0)$ is a cyclic representation of $\mathcal{X}$. Now, if one considers a unital C^*-algebra $\mathcal{X}$ and ρ a state on it then the set

$$\mathcal{L}_\rho := \{B \in \mathcal{X} : \rho(B^*B) = 0\}$$

is a closed subset of $\mathcal{X}$. Furthermore, by Lemma 1.3.3, $\mathcal{X}\mathcal{L}_\rho \subset \mathcal{L}_\rho$. In other words $\mathcal{L}_\rho$ is a closed left-ideal. Then one can define a scalar product on $\mathcal{X}/\mathcal{L}_\rho$ by

$$\left\langle A + \mathcal{L}_\rho, B + \mathcal{L}_\rho \right\rangle_\rho := \rho(A^*B), \qquad A, B \in \mathcal{X}.$$

For any $A \in \mathcal{X}$, one can also define an operator $\tilde{\pi}_\rho(A)$ from $\mathcal{X}/\mathcal{L}_\rho$to itself such that

$$\tilde{\pi}_\rho(A)(B + \mathcal{L}_\rho) := AB + \mathcal{L}_\rho.$$

It is easy to check that $\tilde{\pi}_\rho(A)$ is a linear operator. Moreover, $\tilde{\pi}_\rho(A)$ is bounded. To see this, observe that

$$\|A\|_{\mathcal{X}}^2 B^*B - B^*A^*AB = B^*\left(\|A\|_{\mathcal{X}}^2 \mathbf{1}_{\mathcal{X}} - A^*A\right)B, \quad A, B \in \mathcal{X}.$$

Note also that

$$\|A\|_{\mathcal{X}}^2 \mathbf{1}_{\mathcal{X}} - A^*A = \|A^*A\|_{\mathcal{X}} \mathbf{1}_{\mathcal{X}} - A^*A$$

is a positive element of the C^*-algebra $\mathcal{X}$. Compare with the proof of Lemma 8.1.28 (Appendix 1). Therefore, there exists a (non-trivial) element $C \in \mathcal{X}$ such that

$$\|A^*A\|_{\mathcal{X}}\mathbf{1}_{\mathcal{X}} - A^*A = C^*C.$$

For more details on this aspect, see Section 8.1 (Appendix 1) as well as [26, Theorem 2.2.12]. Then

$$B^*\left(\|A\|_{\mathcal{X}}^2\mathbf{1}_{\mathcal{X}} - A^*A\right)B = B^*C^*CB.$$

Therefore, from the positivity of states of a C^*-algebra, one has

$$\rho(B^*A^*AB) \leq \|A\|_{\mathcal{X}}^2\rho(B^*B).$$

It follows that

$$\|\tilde{\pi}_\rho(A)\|_{\mathcal{X}/\mathcal{L}_\rho} := \sup_{B\in\mathcal{X}/\mathcal{L}_\rho, B\neq 0}\sqrt{\frac{\rho(B^*A^*AB)}{\rho(B^*B)}} \leq \|A\|_{\mathcal{X}}.$$

In other words, $\tilde{\pi}_\rho(A)$ is a bounded linear operator from $\mathcal{X}/\mathcal{L}_\rho$ to itself. Hence, one can define the Hilbert space by:

$$\mathcal{H}_\rho := \overline{\mathcal{X}/\mathcal{L}_\rho}^{\langle\cdot,\cdot\rangle_\rho},$$

a cyclic vector within $\mathcal{H}_\rho$ by

$$A_\rho := (\mathbf{1}_{\mathcal{H}_\rho} + \mathcal{L}_\rho)$$

and finally the map

$$\pi_\rho : \mathcal{X} \to \mathcal{B}(\mathcal{H}_\rho)$$

by using the continuous extension to $\mathcal{H}_\rho$ of the bounded linear operator $\tilde{\pi}_\rho(A)$. Then $(\pi_\rho, \mathcal{H}_\rho, A_\rho)$ is a cyclic representation of $\mathcal{X}$, well-known as the *GNS-representation* (named after I. Gelfand, M. Naimark and I. Segal). For more details on GNS construction, one can see [26, Section 2.3.3]. The *GNS-representation* gives a relation between the algebraic formulation of quantum mechanics and the Hilbert space structure used in Section 1.1.

Chapter 2

Equilibrium State and the 2^{nd} Law of Thermodynamics

In the context of this thesis, we are interested in heat and charge transport properties of *fermions* (like for instance, *electrons*) on a crystal lattice at equilibrium as well as in the derivation of (classical) KMS condition starting from quantum from quantum condition. An important issue to define rigorously a notion of equilibrium state. This is done through the 2^{nd} law of thermodynamics.

2.1 Algebraic Formulation of the 2^{nd} Law of Thermodynamics

In 1824, *N.L.S. Carnot* initiated works on the 2^{nd} *law of thermodynamics*. As it has never failed all along several experiments, it is sometimes qualified as *" one of the most perfect laws of Physics"* (E.H. Lieb and J. Yngvason, 1999), see [50]. To define a state of equilibrium, one can rely on the definition of *entropy*. Here we use the Kelvin-Planck formulation of the 2^{nd} law which uses the concept of *mechanical work*.

Definition 2.1.1 (Kelvin-Planck formulation of the 2^{nd} law of thermodynamics)
Systems in the equilibrium are unable to perform mechanical work in cyclic processes.

Recall that in the algebraic formulation, a state ρ on a generic unital C^*-algebra $\mathcal{X}$ is a continuous, positive and normalized linear functional from $\mathcal{X}$ to $\mathbb{C}$, see Section 1.3. Therefore, to understand this last definition in the context of C^*-algebras, one needs first to define cyclic processes as well as mechanical work. To this end, let $(\mathcal{X}, \tau)$ be a generic C^*-dynamical system. By Definition 1.3.1, recall in this case that $\tau := \{\tau_t\}_{t\in\mathbb{R}}$ is a strongly continuous group of $*$-automorphisms of $\mathcal{X}$. It is generated by an operator δ with domain $\mathcal{D}(\delta) \subseteq \mathcal{X}$. See Section 1.2, for more details about C^*-dynamical systems and Section 8 (Appendix 2) for more details on the (semi)group theory. To implement the notion of mechanical work, we need first to perturb the free time evolution of a quantum system by an external perturbation, which is here switched *on* at a time t_0 (for instance, fix $t_0 = 0$) and switched *off* at a time $T \leq t$. This refers to cyclic processes:

Definition 2.1.2 (Cyclic process)
A process on the physical system in the state ρ at $t = 0$ is defined by a differentiable family $\{A_t\}_{t\geq 0}$ of self-adjoint elements of $\mathcal{X}$. A process $\{A_t\}_{t\geq 0}$ is cyclic with time length $T \geq 0$ if and only if $A_0 = 0$ and $A_t = 0$ for all $t \geq T$.

Then, as we keep observing the system until the time $t \geq T$, we define a strongly continuous two-parameter family $\{\tau_{t,s}\}_{t\geq s}$ of $*$-automorphisms of $\mathcal{X}$ as the solution of a *non-autonomous* evolution equation defined, for any $B \in \mathcal{D}(\delta)$, by

$$\forall t \geq s \geq 0: \quad \partial_t \tau_{t,s}(B) = \tau_{t,s}(\delta(B) + i[A_t, B]), \quad \tau_{s,s}(B) := B\,. \tag{2.1}$$

If the initial state at $t = 0$ is ρ, then the time evolution of the physical system is given by

$$\rho_t = \rho \circ \tau_{t,0}, \qquad t \in \mathbb{R}.$$

We are now in a position to define the mechanical work performed during the time interval $[0, t]$ for any time $t \geq 0$. Indeed, the energy exchanged by a system and its external environment can be defined by (see also [27, lemma 5.4.27]):

Definition 2.1.3 (Energy flux)
The energy exchanged at time $t \geq 0$ between the external device and the physical system perturbed by a process $\{A_t\}_{t\geq 0}$ equals

$$\mathbf{Q}_t^A(\rho) := \int_0^t \rho_s(\partial_s A_s)\,\mathrm{d}s = \int_0^t \rho \circ \tau_{s,0}(\partial_s A_s)\,\mathrm{d}s\,.$$

In particular, if $\mathbf{Q}_t^A(\rho) \geq 0$, then mechanical work is performed on the system. On the other hand when $\mathbf{Q}_t^A(\rho) < 0$, the physical system loses energy. Now, we can reformulate the 2^{nd} law of thermodynamics of Definition 2.1.1 as follows:

Definition 2.1.4 (Algebraic formulation of the 2nd law of thermodynamics)
A state ρ is passive if and only if $\mathbf{Q}_T^A(\rho) \geq 0$ for all cyclic processes $\{A_t\}_{t\geq 0} \subset \mathcal{X}$ of any time length $T \geq 0$.

A minimal requirement for a state ρ to be an equilibrium state is to be stationary, that is in this case,

$$\rho = \rho \circ \tau_t, \quad t \in \mathbb{R}. \tag{2.2}$$

Indeed, in their paper published in 1978, [52, Theorem 1.1], W. Pusz and S.L. Woronowicz set that passive states are invariant under the corresponding autonomous dynamics. Furthermore, following the definition of a passive state and the 2^{nd} law of thermodynamics, a system at thermal equilibrium should not be able to produce work through interaction with any of its copy. In other words, if a system written as $(\mathcal{X}, \tau, \rho)$ is at equilibrium, then the compound system $(\otimes_{j=1}^n \mathcal{X}^{(j)}, \otimes_{j=1}^n \tau^{(j)}, \otimes_{j=1}^n \rho^{(j)})$ (n copies of $(\mathcal{X}, \tau, \rho)$) is also at equilibrium. In fact, $\otimes_{j=1}^n \rho^{(j)}$ is also a passive state for all integer n and it is impossible to extract any energy from the system using cyclic process. This yields the following definition:

Definition 2.1.5 (Completely passive state)
A state ρ is completely passive if only if $\otimes_{j=1}^{n}\rho$ is a passive state of $(\otimes_{j=1}^{n}\mathcal{X}^{(j)}, \otimes_{j=1}^{n}\tau^{(j)})$ for all $n \in \mathbb{N}$. A completely passive state ρ is a thermal equilibrium state of $(\mathcal{X}, \tau)$.

An explicit characterization of thermal equilibrium states has been given by W. Pusz and S.L. Woronowicz in 1978. To introduce that, we need first to say some words about the so-called *Kubo-Martin-Schwinger (KMS)* states. Those states were firstly introduced in 1957 by R. Kubo and in 1959 by P.C. Martin and J. Schwinger. They give a generalization of Gibbs states and they are usually considered as the equilibrium states in the literature.

2.2 Kubo-Martin-Schwinger States and the 2^{nd} Law of Thermodynamics

Recall that $(\mathcal{X}, \tau)$ is an autonomous C^*-dynamical system and define

$$C_0^\infty(\mathbb{R};\mathbb{C}) := \{f \in C^\infty(\mathbb{R};\mathbb{C}) : \exists M \in \mathbb{R}^+ \text{ such that, for } |x| > M,\ f(x) = 0\}$$

to be the space of smooth, compactly supported complex function of the real line. As is usual, we define the Fourier-Laplace transform of a function $f \in C_0^\infty(\mathbb{R};\mathbb{C})$ by

$$\hat{f}(\xi) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-i\xi t} f(t)\mathrm{d}t, \quad \xi \in \mathbb{C}.$$

For $A \in \mathcal{X}$ and $f \in C_0^\infty(\mathbb{R};\mathbb{C})$, define the function $F_{A,f} : \mathbb{C} \to \mathcal{X}$ by

$$F_{A,f}(z) := \int_{-\infty}^{+\infty} \hat{f}(t-z)\tau_t(A)\mathrm{d}t$$

as well as the dense subspace

$$\mathcal{X}_\tau := \{A_f := F_{A,f}(0) : A \in \mathcal{X},\ f \in C_0^\infty(\mathbb{R};\mathbb{C})\}.$$

Since $f \in C_0^\infty(\mathbb{R};\mathbb{C})$, note that by the Paley Wiener Theorem, see [55, Theorem 19.3], $\hat{f}$ is an analytic function on $\mathbb{C}$. Moreover, τ is a $*$-automorphism. Therefore, $F_{A,f}$ is differentiable in any $z \in \mathbb{C}$. Observe that, for all $t \in \mathbb{R}$,

$$F_{A,f}(t) = F_{\tau_t(A),f}(0) = \tau_t\left(F_{A,f}(0)\right) = \tau_t(A_f).$$

For all $A_f \in \mathcal{X}_\tau$ and $z \in \mathbb{C}$, define $\tau_z(A_f) =: F_{A,f}(z)$. The map $z \mapsto \tau_z(A_f)$ is analytic on $\mathbb{C}$ and $\tau_z(A_f) = \tau_t(A_f)$ for $z = t \in \mathbb{R}$ (uniqueness of analytic expansion). We are now in a position to define the so-called *KMS* states.

Definition 2.2.1 (KMS states)
Recall that $(\mathcal{X}, \tau)$ is an autonomous C^*-dynamical system and $\beta := T^{-1} > 0$ be the so-called inverse temperature. A state ρ is said to be a (τ, β)-KMS state when, for all $A \in \mathcal{X}$ and $B \in \mathcal{X}_\tau$,

$$\rho(A\tau_{i\beta}(B)) = \rho(BA).$$

An example of KMS state can easily be constructed, for instance on $\mathcal{X} = \mathcal{B}(\mathcal{H})$: Let $H \in \mathcal{B}(\mathcal{H})$ be a self adjoint element of a C^*-algebra $\mathcal{X}$. If $\tau := \{\tau_t\}_{t\in\mathbb{R}}$ is defined by

$$\tau_t(B) := \mathrm{e}^{itH} B \mathrm{e}^{-itH}, \qquad B \in \mathcal{X},\ t \in \mathbb{R},$$

then $(\mathcal{X}, \tau)$ is a C^*-dynamical system. If $\mathcal{X} = \mathcal{B}(\mathcal{H})$ and $\mathrm{e}^{-\beta H}$ is a trace-class operator on $\mathcal{H}$, for $\beta > 0$, then we define

$$C := \frac{\mathrm{e}^{-\beta H}}{\mathrm{trace}\,(\mathrm{e}^{-\beta H})} \in \mathcal{B}(\mathcal{H}).$$

By a straightforward computations, it is easy to see that the state ρ_C, well-known as a Gibbs state, defined by

$$\rho_C(B) := \mathrm{trace}(CB), \quad \forall B \in \mathcal{B}(\mathcal{H}) \tag{2.3}$$

is a (τ, β)-*KMS* state. We are now in a position to give the explicit characterization of thermal equilibrium states in terms of KMS states, see also [52, Theorem 1.4]:

Theorem 2.2.1 (Pusz-Woronowicz, 1978)
Let $(\mathcal{X}, \tau)$ be a C^*-dynamical system, ρ is a thermal equilibrium state of $(\mathcal{X}, \tau)$ if and only if it is a (stationary) (τ, β)-KMS state of $(\mathcal{X}, \tau)$ for some $\beta \in [0, \infty]$.

Within the following section, we characterize the quantum fundamental particles that are *bosons* and *fermions*. This will lead us to a more precise definition of the framework of this thesis such as the C^*-algebras which will be involved, the spatial framework, etc...

Chapter 3

Quantum Many-Body Problem

A standard characteristic of Quantum Fields Theory (QFT) is that the number of particles is not given as an hypothesis. In other words, instead of considering a fix number of particles (such as it is done in Equations (1.1)-(1.2)), one needs a framework that takes into account at once all possible particle numbers. This is related to the celebrated *Fock space* representation of the quantum many-body problem, which is given here for pedagogical reasons in order to present afterwards the algebraic formulation of quantum many-body problems.

3.1 The Fock Space Representation

3.1.1 The Fock space

In this part, for the sake of clarity, we rely again on the concept of wave functions, which are represented by a family $\{\psi(t)\}_{t\in\mathbb{R}}$ within a Hilbert space $\mathfrak{h}$ with scalar product denoted by $\langle\cdot,\cdot\rangle_{\mathfrak{h}}$. Then, the description of n-particles involves the Hilbert space

$$\mathfrak{h}^n := \mathfrak{h} \otimes ... \otimes \mathfrak{h},$$

which, for $n \in \mathbb{N}$, is the n-tensor product of the same Hilbert space $\mathfrak{h}$. For more details on tensor products of Hilbert spaces, see [53, section II.4]. This allows to deal with the so-called case of *many-body problem*. As previously explained, instead of taking a fix number of particles as a given hypothesis, n is taken as a variable, which could thus be an arbitrary *huge* integer. From this, and by using the term *wave functions* mentioned above, one then works with vectors of the following Hilbert space:

$$\mathfrak{F}(\mathfrak{h}) := \bigoplus_{n\geq 0} \mathfrak{h}^n \tag{3.1}$$

with $\mathfrak{h}^0 := \mathbb{C}$ and scalar product given by

$$\langle\psi,\varphi\rangle_{\mathfrak{F}(\mathfrak{h})} = \langle\psi^{(0)},\varphi^{(0)}\rangle_{\mathbb{C}} + \sum_{n\geq 1}\langle\psi^{(n)},\varphi^{(n)}\rangle_{\mathfrak{h}^n}, \quad \psi,\varphi \in \mathfrak{F}(\mathfrak{h}).$$

This is the celebrated Fock space. Within this formulation, wave functions are described by sequences $\psi = (\psi^{(n)})_{n\geq 0}$, where $\psi^{(n)} \in \mathfrak{h}^n$ for all integer $n \geq 0$. For any $n \geq 0$, the n-tensor product $\mathfrak{h}^n$ of the Hilbert space $\mathfrak{h}$ is seen as a closed subspace of the Fock space, using the canonical identification

$$\psi^{(n)} \equiv \left(0, 0, \cdots, 0, \psi^{(n)}, 0, 0, \cdots\right) \in \mathfrak{F}(\mathfrak{h}).$$

3.1.2 The Fermion and Boson Fock spaces

In this thesis, we consider fermionic and bosonic systems. It means that the wave functions are anti-symmetric in the *fermionic* case and symmetric in the case of *bosons*. This yields a definition of both symmetric and anti-symmetric Fock space. To explain this, let us consider the following operators $P_\pm \in \mathcal{B}(\mathfrak{F}(\mathfrak{h}))$ uniquely defined by the conditions:

$$P_-(f_1 \otimes f_2 \otimes \cdots \otimes f_n) := \frac{1}{n!} \sum_\pi \varepsilon_\pi f_{\pi(1)} \otimes f_{\pi(2)} \otimes \cdots \otimes f_{\pi(n)}, \tag{3.2}$$

$$P_+(f_1 \otimes f_2 \otimes \cdots \otimes f_n) := \frac{1}{n!} \sum_\pi f_{\pi(1)} \otimes f_{\pi(2)} \otimes \cdots \otimes f_{\pi(n)}, \tag{3.3}$$

for all $n \in \mathbb{N}$ and $f_i \in \mathfrak{h}$ for $i = 1, ..., n$. In Equations (3.2)-(3.3), π is any permutation with a signature $\varepsilon_\pi \in \{-1, 1\}$:

$$\pi : (1, 2, 3, \cdots, n) \to (\pi(1), \pi(2), \pi(3), \cdots, \pi(n)).$$

The index "+" stands for *bosons* while the "−" sign stands for *fermions*. By straightforward computations, one can see that the operators $P_\pm$ are orthogonal projections. We define the *bosonic* and *fermionic* Fock space respectively by

$$\mathfrak{F}_\pm(\mathfrak{h}) := P_\pm \mathfrak{F}(\mathfrak{h}) = \bigoplus_{n\geq 0} P_\pm \mathfrak{h}^n.$$

Clearly, its corresponding n-particle subspace is given by

$$\mathfrak{h}^n_\pm := P_\pm \mathfrak{h}^n.$$

They are again seen as subspaces of $\mathfrak{F}_\pm(\mathfrak{h})$, $P_+\mathfrak{h}^n$ being the n-boson Hilbert space while $P_-\mathfrak{h}^n$ is the n-fermion one.

Remark 3.1.1 (Vacuum state)
The trivial case where there is no particle (0-particle) is described from the vacuum state $(1, 0, 0, \ldots)$.

In order to understand the use of the orthogonal projections $P_\pm$ and the physical meaning of the (anti-) symmetry properties of the wave functions describing n-particles ($n \in \mathbb{N}$), let us consider the Hilbert space of square integrable functions on $\mathbb{K} = \mathbb{R}^d, \mathbb{Z}^d$

($d \in \mathbb{N}$) as the one-particle Hilbert space $\mathfrak{h}$. In this case, at the microscopic scale, identical particles are not distinguishable. This fact is well-described by the symmetry (under any permutation of particles) of $|\psi^{(n)}(x_1, \cdots, x_n)|^2$. Indeed, considering $n \in \mathbb{N}$ identical particles and $1 \leq i < j \leq n$, one has:

$$|\psi^{(n)}(x_1, \cdots, x_i, \cdots, x_j, \cdots, x_n)|^2 = |\psi^{(n)}(x_1, \cdots, x_j, \cdots, x_i, \cdots, x_n)|^2.$$

This is the probability to find n-particles at positions $x_1, \cdots, x_i, \cdots, x_j, \cdots, x_n \in \mathbb{K}$. Two types of particle arise here: a first type when the components $\psi^{(n)}$ are symmetric under a permutation of coordinates and a second one for anti-symmetric components under a permutation of coordinates. A particle that belongs to the first category is called *boson*, while in the second one the particles are called *fermions*. In a more abstract framework, such a property are reflected by the n-particles Hilbert space $P_\pm \mathfrak{h}^n$: $P_+ \mathfrak{h}^n$ is n-boson Hilbert space while $P_- \mathfrak{h}^n$ is n-fermion one, as already explained.

Remark 3.1.2 (Pauli exclusion principle)
Assume that $\mathfrak{h}$ the Hilbert space of square integrable functions on $\mathbb{K} = \mathbb{R}^d, \mathbb{Z}^d$. Take two fermions with wave function[1] $\psi \in P_- \mathfrak{h}^n$. *Then, for any $x_1, x_2 \in \mathbb{K}$,*

$$\psi(x_1, x_2) = -\psi(x_2, x_1). \tag{3.4}$$

In particular, $\psi(x, x) = 0$ whenever $x_1 = x_2 = x$. In other words, two fermions cannot exactly be at the same position. This is a consequence of the celebrated Pauli exclusion principle. This fact will also be reflected by the CAR C^*-algebra described later.

3.1.3 The second quantization

An operator h on a one-particle Hilbert space $\mathfrak{h}$ can naturally be extended to the whole bosonic or fermionic Fock space $\mathfrak{F}_\pm(\mathfrak{h})$. This refers to the *second quantization* of the operator h, which is denoted by $d\Gamma(h)$. This process is particularly interesting for self-ajoint operators, which represent *observables* in quantum mechanics.

Consider a self-adjoint operator h acting on $\mathfrak{h}$. Its domain denoted by $\mathcal{D}(h)$. One can define an operator h_n acting on $\mathfrak{h}_\pm^n$ with domain $\mathcal{D}(h_n) \supseteq \mathcal{D}(h)^n$ ($\mathcal{D}(h)^0 := \mathbb{C}$, $\mathcal{D}(h_n)$ is a continuous extension of $\mathcal{D}(h)^n$) such that

$$\begin{aligned} h_0 &= 0, \\ h_n(P_\pm(f_1 \otimes f_2 \otimes \cdots \otimes f_n)) &= P_\pm \textstyle\sum_{i=1}^n (f_1 \otimes f_2 \otimes h f_i \otimes \cdot \otimes \cdots \otimes f_n). \end{aligned} \tag{3.5}$$

for all $i = 1, ..., n$, $f_i \in \mathcal{D}(h)$. Consider now the operator defined by

$$d\Gamma_0(h) := \bigoplus_{n \geq 0} h_n.$$

[1]Note that we have dropped the time component $t \in \mathbb{R}$ on purpose since this is non relevant to describe *bosons* and *fermions*.

Its domain is given by

$$\mathcal{D}(d\Gamma_0(h)) := \left\{(\psi^{(n)})_{n\in\mathbb{N}} \in \mathfrak{F}_\pm(\mathfrak{h}) : \psi^{(n)} \in \mathcal{D}(h_n),\ \exists\, N \in \mathbb{N},\ \psi^{(n)} = 0,\ n \geq N\right\}.$$

First, note that h_n and thus its direct sum are symmetric operators and hence, closable. Moreover, by construction of the Fock space, $\mathcal{D}(d\Gamma_0(h))$ contains a dense set of analytic vectors in $\mathfrak{F}_\pm(\mathfrak{h})$, which is formed by finite sums of (anti-) symmetrized products of analytic vectors of h. Therefore, one can define the self-adjoint closure of $d\Gamma_0(h)$ by

$$d\Gamma(h) := \overline{d\Gamma_0(h)}.$$

$d\Gamma(h)$ is a natural extension of h to the whole bosonic or fermionic Fock space $\mathfrak{F}_\pm(\mathfrak{h})$ and is called the *second quantization* of h. This notion will appear to be very useful in the sequel.

As an example, consider the identity operator of $\mathfrak{h}$ denoted by $\mathbf{1}_\mathfrak{h}$. Then, we directly deduce from (3.5) that, for any integer $n \geq 0$,

$$(\mathbf{1}_\mathfrak{h})_n = P_\pm n(\mathbf{1}_\mathfrak{h} \otimes \mathbf{1}_\mathfrak{h} \otimes ... \otimes \mathbf{1}_\mathfrak{h}) = nP_\pm \mathbf{1}_{\mathfrak{h}^n}. \tag{3.6}$$

For this reason, the second quantization of $\mathbf{1}_\mathfrak{h}$, denoted by $d\Gamma(\mathbf{1}_\mathfrak{h})$, is naturally called the *particle number operator*. For more details about the structure of Fock spaces, see [27, section 5.2.1].

3.1.4 Annihilation and creation operators

In the context of this thesis, the operator $d\Gamma(\cdot)$ described above turns out to be more intuitive through its algebraic formulation by using the so-called *annihilation* and *creation* operators. This will be explained in this section and will lead to the algebraic formulation of quantum many-body problems.

Definition 3.1.3 (Annihilation/creation operators)
For $f \in \mathfrak{h}$, we define the operators $a(f)$ and $a^*(f)$ acting on $\mathfrak{F}(\mathfrak{h})$, respectively called annihilation and creation operators, as follows: $a(f)\psi^{(0)} = 0$, $a^*(f)\psi^{(0)} = f$, for any $\psi^{(0)} \in \mathfrak{h}^0$, and for any $n \in \mathbb{N}$, $f_1, ..., f_n \in \mathfrak{h}$,

$$a(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_n)) = n^{\frac{1}{2}}(f, f_1) f_2 \otimes f_3 \otimes \cdots \otimes f_n,$$
$$a^*(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_n)) = (n+1)^{\frac{1}{2}} f \otimes f_1 \otimes \cdots \otimes f_n.$$

Note that, by [27, section 5.2.1], for $f \in \mathfrak{h}$, $a^*(f)$ is the adjoint operator of $a(f)$. This relation also holds for the *annihilation* and *creation* operators $a_\pm(f)$ and $a_\pm^*(f)$ on the bosonic and fermionic Fock spaces defined by

$$a_\pm(f) = P_\pm\, a(f)\, P_\pm, \quad a_\pm^*(f) = P_\pm\, a^*(f)\, P_\pm.$$

where the operators P_+, P_- are the orthogonal projections respectively defined by Equation (3.2) and Equation (3.3). Recall that, for two linear operators A and B acting on a Hilbert space,

$$\{A, B\} := AB - BA \quad \text{and} \quad [A, B] := AB - BA.$$

Then a direct computation leads to

$$[a_+(f), a_+(g)] = [a_+^*(f), a_+^*(g)] = 0 \quad \text{and} \quad [a_+(f), a_+^*(g)] = \langle f, g\rangle_{\mathfrak{h}} \mathbf{1}_{\mathfrak{F}_+(\mathfrak{h})}. \tag{3.7}$$

The above relations are well-known in the literature and are called *canonical commutation relations* (CCR). Meanwhile,

$$\{a_-(f), a_-(g)\} = \{a_-^*(f), a_-^*(g)\} = 0 \quad \text{and} \quad \{a_-(f), a_-^*(g)\} = \langle f, g\rangle_{\mathfrak{h}} \mathbf{1}_{\mathfrak{F}_-(\mathfrak{h})}. \tag{3.8}$$

The above relations are also well-known and are called *canonical anti-commutation relations* (CAR).

Remark 3.1.4 (Notations)
From now, to simplify the notation, we will drop the " $\pm$ " index of $P_\pm$, $a_\pm(\cdot)$, $a_\pm^*(\cdot)$, $\mathfrak{h}$ and $\mathfrak{F}_\pm(\mathfrak{h})$. We define $a(\cdot) := a_\pm(\cdot)$, $a^*(\cdot) := a_\pm^*(\cdot)$, $\mathfrak{h}^n := \mathfrak{h}_\pm^n$, for all $n \geq 0$. Finally, $\mathfrak{F}(\mathfrak{h}) := \mathfrak{F}_\pm(\mathfrak{h})$ refers either to the bosonic Fock space or the fermionic Fock space, depending whether we deal with bosons or fermions.

3.1.5 Consequences of CAR relations

The first important consequence of CAR relations (3.8) are the fact that the fermionic annihilation and creation operators are bounded:

Proposition 3.1.5 (Norm of fermionic annihilation/creation operators)
Let $\mathfrak{h}$ be a Hilbert space, $\mathfrak{F}(\mathfrak{h})$ the fermionic Fock space and $a(f)$, $a^*(f)$ its corresponding annihilation and creation operator, respectively. Then, for all $f \in \mathfrak{h}$,

$$\|a(f)\|_{\mathcal{B}(\mathfrak{F}(\mathfrak{h}))} = \|a^*(f)\|_{\mathcal{B}(\mathfrak{F}(\mathfrak{h}))} = \|f\|_{\mathfrak{h}},$$

i.e the annihilation and creation operators have bounded extensions.

Proof: By using the CAR, one can easily check that

$$\begin{aligned}(a^*(f)a(f))^2 &= a^*(f)\,\{a(f), a^*(f)\}\,a(f)\\ &= \|f\|_{\mathfrak{h}}^2 a^*(f)a(f).\end{aligned}$$

Then,

$$\begin{aligned}\|a(f)\|_{\mathcal{B}(\mathfrak{F}(\mathfrak{h}))}^4 &= \|\,(a^*(f)a(f))^2\,\|_{\mathcal{B}(\mathfrak{F}(\mathfrak{h}))}\\ &= \|f\|_{\mathfrak{h}}^2 \|a^*(f)a(f)\|_{\mathcal{B}(\mathfrak{F}(\mathfrak{h}))}\\ &= \|f\|_{\mathfrak{h}}^2 \|a(f)\|_{\mathcal{B}(\mathfrak{F}(\mathfrak{h}))}^2\end{aligned}$$

which yields the assertion, using that $a(f) \neq 0$ for $f \neq 0$. ■

Obviously, the map $f \mapsto a(f)$ from $\mathfrak{h}$ to $\mathcal{B}(\mathfrak{F}(\mathfrak{h}))$ is anti-linear, while the map $f \mapsto a^*(f)$ from $\mathfrak{h}$ to $\mathcal{B}(\mathfrak{F}(\mathfrak{h}))$ is linear. In Remark 3.1.2, we have seen that one characterization of *fermions* is the Pauli exclusion principle. This property arises naturally as a consequence of the *canonical anti-commutation relations* (CAR), see (3.8). Recall that here we dropped the index " − ", for the annihilation/creation of *fermions*. Let the *vacuum* (0-particle state) be $\Omega = (1, 0, 0, ...)$, see Remark 3.1.1. Then

$$a^*(f)\Omega$$

creates a *fermion* in the state f, i.e. it maps the vacuum to a one-particle wave function $f \in \mathfrak{h}$. In the same way, the operator defined by

$$(n!)^{\frac{1}{2}} a^*(f_1)...a^*(f_n)\Omega = P_-(f_1 \otimes ... \otimes f_n) \tag{3.9}$$

creates successively n-particles in the states $f_1, ..., f_n \in \mathfrak{h}$, for $n \in \mathbb{N}$. In the opposite way, $a(f)$ reduces the number of particles, this explains the naming *annihilation* and *creation* operators. But, by anti-symmetry, if $f_i = f_j$ for $i \neq j$, then

$$P_-(f_1 \otimes ... \otimes f_n) = 0.$$

Therefore, it is not allowed to create two fermions exactly in the same state. We recover the Pauli exclusion principle explained in a special example in Remark 3.1.2.

3.1.6 Consequences of CCR relations and Weyl operators

As we have just seen above, in the case of *fermions*, because of the signature ε_π of P_-, see Equation (3.2), one deals with anti-symmetric functions. This is related to the Pauli exclusion principle and the fermionic annihilation/creation operators are bounded, see Proposition 3.1.5. By contrast, *bosons* do not satisfy the Pauli exclusion principle and they can accumulate in a given state. This is related to the fact that the annihilation/creation operators of *bosons* are unbounded. It is thus natural to introduce the unitary operators, the so-called *Weyl operators*, generated by self-adjoint combination of annihilation/creation operators of bosons. To present that, recall here that $a(\cdot) := a_+(\cdot)$, $a^*(\cdot) := a_+^*(\cdot)$, $\mathfrak{h}^n := \mathfrak{h}_+^n$, for all $n \geq 0$, and $\mathfrak{F}(\mathfrak{h}) := \mathfrak{F}_+(\mathfrak{h})$. The fields operators are defined as follows:

Definition 3.1.6 (Field operators)
For $f \in \mathfrak{h}$, the boson field operator is the (unbounded) self-adjoint operator defined by

$$\Phi(f) := \frac{1}{\sqrt{2}} \left(a\left(f\right) + a^*\left(f\right) \right) := \frac{1}{\sqrt{2}} \Re\mathrm{e}\left(a\left(f\right) \right).$$

(One can define in the same way a field operator as the imaginary part of $a\left(f\right)$, or use $\Phi(if)$).

Define the set

$$\mathfrak{F}_0 := \left\{ (\psi^{(n)})_{n\in\mathbb{N}} \in \mathfrak{F}(\mathfrak{h}) : \exists\, N \in \mathbb{N},\, \psi^{(n)} = 0,\, n \geq N \right\},$$

which, by construction of the boson Fock space, is a dense subset of $\mathfrak{F}(\mathfrak{h})$. By [27, Proposition 5.2.3], for any $f \in \mathfrak{h}$, $\Phi(f)$ is essentially self-adjoint on $\mathfrak{F}_0$ and we denote its self-adjoint extension again by $\Phi(f)$. Because of the unboundedness of the annihilation/creation operators, for the technical computations, one considers the unitary operators

$$W(f) := \mathrm{e}^{i\Phi(f)}, \quad f \in \mathfrak{h}.$$

These are called the Weyl operators. They satisfy the so-called Weyl form of canonical commutation relations (CCR), see [27, Section 5.2.2.2], that is:

$$W(f)W(g) = \mathrm{e}^{\frac{-i\,\mathrm{Im}}{2}\langle f,g\rangle_{\mathfrak{h}}} W(f+g) = \mathrm{e}^{-i\,\mathrm{Im}\,\langle f,g\rangle_{\mathfrak{h}}} W(g)W(f), \quad f,g \in \mathfrak{h}.$$

3.1.7 The second quantization in terms of annihilation/creation operators

At this point, we do not really see exactly the structure of self-adjoint operators or *observables*. In order to fill this gap and to define particular physical quantities, we first give some intuition and use the celebrated *second quantization* of one-particle operators that we have already defined. Through this, we will see that the annihilation/creation operators appear naturally to describe a physical system. Since the computations are basically the same for the bosonic or fermionic cases, we will only do the computations for *fermions*.

Proposition 3.1.7 (Algebraic second quantization)
Let h be a self-adjoint operator acting on $\mathfrak{h}$ such that its orthonormal basis is given by $\{\mathfrak{e}_i\}_{i\in I}$. Therefore, the second quantization of h is

$$d\Gamma(h) = \sum_{j,k\in I} \left\langle \mathfrak{e}_k, h\, \mathfrak{e}_j \right\rangle_{\mathfrak{h}} a^*(\mathfrak{e}_k) a(\mathfrak{e}_j). \tag{3.10}$$

Proof: The proof is given for the case of *fermions*, the bosonic case being identical. Recall Notation 3.1.4. For any integer n, recall that the n-patricle Hilbert space $\mathfrak{h}^n$ is the n-tensor product of $\mathfrak{h}$ and let h_n be the operator acting on $\mathfrak{h}^n$ given by (3.5). For any, $\psi^{(n)} \in \mathfrak{h}^n_- = P_-\mathfrak{h}^n$

$$h_n\psi^{(n)} = h_n P_- \psi^{(n)} = P_- h_n P_- \psi^{(n)}$$

with P_- being the orthogonal projection defined by Equation (3.2). In particular, for any index $i \in \{1, ..., n\}$,

$$P_-(\mathbf{1}_{\mathfrak{h}_1} \otimes \mathbf{1}_{\mathfrak{h}_2} \otimes ... \otimes \mathbf{1}_{\mathfrak{h}_{i-1}} \otimes h \otimes \mathbf{1}_{\mathfrak{h}_{i+1}} \otimes ... \otimes \mathbf{1}_{\mathfrak{h}_n})P_- = P_-(h \otimes \mathbf{1}_{\mathfrak{h}_2} \otimes ... \otimes \mathbf{1}_{\mathfrak{h}_n})P_-$$

where $\mathfrak{h}_i = \mathfrak{h}$ for all $i \in \{1, ..., n\}$ and $\mathbf{1}_\mathfrak{h}$ is the identity map of $\mathfrak{h}$. Therefore,

$$h_n \psi^{(n)} = n\, P_-(h \otimes \mathbf{1}_{\mathfrak{h}_2} \otimes ... \otimes \mathbf{1}_{\mathfrak{h}_n})\psi^{(n)}.$$

Assume without loss of generality that

$$\psi^{(n)} = \frac{1}{n!} \sum_{\pi \in S_n} \varepsilon_\pi \varphi_{\pi(1)} \otimes ... \otimes \varphi_{\pi(n)}$$

with $\varphi_1, ..., \varphi_1 \in \mathfrak{h}$. Recall that $\varepsilon_\pi = \{-1, 1\}$ is the signature of any permutation $\pi \in S_n$ of $\{1, \ldots, n\}$. By using *Dirac notation*, in particular the notation $|\varphi\rangle\langle\varphi|$ for the orthogonal projection onto the vector subspace spanned by $\varphi \in \mathfrak{h}$, if the family $\{\mathfrak{e}_j\}_{j \in I}$ is the orthonormal basis of $\mathfrak{h}$, then observe that, of course,

$$\sum_{j \in I} |\mathfrak{e}_j\rangle\langle\mathfrak{e}_j| = \mathbf{1}_\mathfrak{h}.$$

A direct computation yields that

$$h_n(P_-\psi^{(n)}) = \sqrt{n} \sum_{j,k \in I} \left\langle \mathfrak{e}_k, h\mathfrak{e}_j \right\rangle_\mathfrak{h} P_- \left(\mathfrak{e}_k \otimes \frac{1}{n!} \sum_{\pi \in S_n} \varepsilon_\pi \left(\sqrt{n} \left\langle \mathfrak{e}_j, \varphi_{\pi(1)} \right\rangle_\mathfrak{h} \varphi_{\pi(2)} \otimes ... \otimes \varphi_{\pi(n)} \right) \right).$$

By using Equation (3.9) and the definition of *creation/annihilation* operators on the fermion Fock space (Definition 3.1.3), one has

$$h_n \psi^{(n)} = \sqrt{n} \sum_{j,k \in I} \left\langle \mathfrak{e}_k, h\mathfrak{e}_j \right\rangle_\mathfrak{h} P_- \left(\mathfrak{e}_k \otimes a(\mathfrak{e}_j) \right) \psi^{(n)} = \left(\sum_{j,k \in I} \left\langle \mathfrak{e}_k, h\mathfrak{e}_j \right\rangle_\mathfrak{h} a^*(\mathfrak{e}_k) a(\mathfrak{e}_j) \right) \psi^{(n)}.$$

This concludes the proof. ■

Recall that the *observables* in a C^*-algebra are self-adjoint elements acting on some Hilbert space, see Section 1.3. Within the next section we will develop this part with the algebraic formulation of quantum many-body problems. Nevertheless, since in the first part of the thesis, the results were obtained in the context of *fermions*, from now we consider the case of fermionic annihilation/creation operators satisfying (3.8). We will introduce the bosonic case when it is required.

3.2 Algebraic Formulation of Fermionic Systems

We present hereby the algebraic formulation of fermionic systems since the thesis predominantly study such quantum systems. The same kind of mathematical development can be done for bosonic systems, by using the CCR C^*-algebra constructed from the Weyl operators, instead.

3.2.1 CAR Algebras

As explained in previous sections, the so-called creation/annihilation operators, indexed by elements of the one-particle Hilbert space $\mathfrak{h}$, acting on the Fermion Fock space are very useful to define many-fermion systems. See for instance Proposition 3.1.7. This leads to consider the so-called CAR algebra defined as follows:

Definition 3.2.1 (CAR C^*-algebra)
The CAR algebra

$$\mathcal{U} \equiv \mathrm{CAR}(\mathfrak{h}) \equiv (\mathrm{CAR}(\mathfrak{h}), +, \cdot, *) \tag{3.11}$$

associated with the Hilbert space $\mathfrak{h}$ *is the* C^**-algebra generated by a unit* $\mathbf{1}$ *and a family* $\{a(\psi)\}_{\psi\in\mathfrak{h}}$ *of elements satisfying Conditions (a)-(b):*
(a) *The map* $f \mapsto a(\psi)^*$ *is (complex) linear.*
(b) *The family* $\{a(\psi)\}_{\psi\in\mathfrak{h}}$ *satisfies the CAR: For all* $\psi, \varphi \in \mathfrak{h}$*,*

$$\{a(\psi), a(\varphi)\} = 0 \quad \textit{and} \quad \{a(\psi), a^*(\varphi)\} = \langle \psi, \varphi \rangle_{\mathfrak{h}} \mathbf{1}. \tag{3.12}$$

Strictly speaking, the above conditions (a)-(b) only define $\mathcal{U}$ up to an isomorphism of C^*-algebra [27, Theorem 5.2.5]. In Physics, the generator $a(\varphi) \in \mathcal{U}$ is the annihilation operator associated with the one-particle wave function $\varphi \in \mathfrak{h}$ whereas its adjoint $a(\varphi)^*$ is the corresponding creation operator: The CAR (3.12) is equivalent to (3.8) in the Fock space representation and implements the Pauli exclusion principle. More precisely, by defining the Fock representation $\pi : \mathcal{U} \to \mathcal{B}(\mathfrak{F}_-(\mathfrak{h}))$ as the unique $*$-morphism mapping $a(\psi) \in \mathcal{U}$ to the annihilation operator $\pi(a(\psi)) \equiv a_-(\psi) \in \mathcal{B}(\mathfrak{F}_-(\mathfrak{h}))$ of Definition 3.1.3. If $\mathfrak{h}$ is finite-dimensional then $\mathfrak{F}_-(\mathfrak{h})$ is also finite-dimensional, by antisymmetry of waves functions. In this case, the Fock representation is faithfull and so,

$$\pi(\mathcal{U}) = \mathcal{B}(\mathfrak{F}_-(\mathfrak{h})) . \tag{3.13}$$

The CAR algebra $\mathcal{U}$ becomes really pivotal when the Hilbert space $\mathfrak{h}$ is infinite-dimensional. In this case, (3.13) does not hold true anymore and

$$\pi(\mathcal{U}) \subsetneq \mathcal{B}(\mathfrak{F}_-(\mathfrak{h})) . \tag{3.14}$$

See, e.g., [31, Lemma 3.4]. In fact, in this case, the algebraic approach is more general than the Hilbert space based approach because of the non-uniqueness of irreducible representations. In Physics, this is intimately related to the existence of various thermodynamically stable phases of the same material. See explanation of [31, Section 2.6] for more details.

3.2.2 Bilinear elements

From Equation (3.10), the *second quantization* obtained from operators acting on a Hilbert space are "some" 2-degrees polynomial in $a(\cdot)$ and $a^*(\cdot)$. See for instance Proposition 3.1.7. We give a more general definition of those elements, also called *bilinear elements*, a term introduced by H. Araki at the end of the sixties. Recall that we focus here on the fermionic framework for which the annihilation/creation operators satisfy (3.12).

Definition 3.2.2 (Bilinear elements)
For an operator $C \in \mathcal{B}(\mathfrak{h})$, consider a finite dimensional subspace $\mathcal{H} \subset \mathfrak{h}$ with orthonormal basis $\{\psi_i\}_{i\in I}$, such that $\operatorname{ran}(C) \subseteq \mathcal{H}$ and $\operatorname{ran}(C^*) \subseteq \mathcal{H}$. We define the bilinear element associated with C to be

$$\langle \mathrm{A}, C\mathrm{A}\rangle := \sum_{i,j\in I} \left\langle \psi_i, C\psi_j \right\rangle_{\mathfrak{h}} a\left(\psi_i\right)^* a\left(\psi_j\right).$$

Note that such a finite dimensional $\mathcal{H}$ in this definition always exists, because

$$\dim\left(\operatorname{ran}(C)\right) = \dim\left(\operatorname{ran}(C^*)\right) < \infty,$$

and is an invariant space of C containing $(\ker(C))^{\perp}$. Hence, $\langle \mathrm{A}, C\mathrm{A}\rangle$ does not depend on the particular choice of $\mathcal{H}$ and its orthonormal basis. It is also useful to mention that the adjoint of $\langle \mathrm{A}, C\mathrm{A}\rangle$ is

$$\langle \mathrm{A}, C\mathrm{A}\rangle^* = \langle \mathrm{A}, C^*\mathrm{A}\rangle. \tag{3.15}$$

In particular, a bilinear element is an *observable* when it is the *second quantization* of self-adjoint, finite range operator in $\mathcal{B}(\mathfrak{h})$, as expected. See again Proposition 3.1.7. (Recall the definition of an *observable* in a C^*-algebra in section 1.3). Additionally, for B in any generic C^*-algebra $\mathcal{X}$, we define its real and imaginary parts respectively by

$$\Re\mathrm{e}(B) = \frac{1}{2}\left(B + B^*\right) \quad \text{and} \quad \Im\mathrm{m}(B) = \frac{1}{2i}\left(B - B^*\right).$$

A straightforward computation yields

$$\Im\mathrm{m}\left\{\langle \mathrm{A}, C\mathrm{A}\rangle\right\} = \langle \mathrm{A}, \Im\mathrm{m}\left\{C\right\}\mathrm{A}\rangle \quad \text{and} \quad \Re\mathrm{e}\left\{\langle \mathrm{A}, C\mathrm{A}\rangle\right\} = \langle \mathrm{A}, \Re\mathrm{e}\left\{C\right\}\mathrm{A}\rangle. \tag{3.16}$$

A particular self-adjoint bilinear element is defined to be the so-called *Hamiltonian* which is associated with the energy *observable* of the physical system under consideration.

Definition 3.2.3 (Bilinear hamiltonian)
Given an orthonormal basis $\{\psi_i\}_{i\in I}$ of finite-dimensional Hilbert space $\mathcal{H} \subset \mathfrak{h}$ and a self-adjoint operator $h \in \mathcal{B}(\mathcal{H})$ whose range is finite-dimensional, we define the bilinear Hamiltonian by

$$\langle \mathrm{A}, h\mathrm{A}\rangle := \sum_{i,j\in I} \left\langle \psi_i, h\psi_j \right\rangle_{\mathfrak{h}} a\left(\psi_i\right)^* a\left(\psi_j\right).$$

A particular property of *bilinear elements* is associated to the so-called *quasi-free dynamics* that we are going to explain in detail in the next section.

3.2.3 Quasi-free dynamics

As we already mentioned from the beginning, the time evolution of the quantum system is given by some specific strongly continuous group of $*$-automorphisms. In the context of this work, the dynamic has a specific property. They are constructed from *Bogoliubov*

$*$-automorphisms, as described in [5], and the dynamics is named *quasi-free* because it is generated by bilinear Hamiltonians, i.e., by the second quantization of a one-particle Hamiltonian. In order to give a definition of those dynamics, we give a first observation on the commutator of bilinear elements (Definition 3.2.2) with the generators $\{a(f), a^*(f),\ f \in \mathfrak{h}\}$ of the CAR C^*-algebra $\mathcal{U}$. Note that here, once again, the annihilation/creation operators satisfy the CAR properties (3.8). Recall also that $\mathcal{B}(\mathfrak{h})$ denotes the Banach space of all bounded (linear) operators acting on the (one-particle) Hilbert space $\mathfrak{h}$.

Proposition 3.2.4 (Monomial commutation with a bilinear element)
For any $C \in \mathcal{B}(\mathfrak{h})$ whose range is finite-dimensional and for any $\varphi \in \mathfrak{h}$, one has

$$[\langle \mathrm{A}, \mathrm{CA}\rangle, a(\varphi)] = -a(\mathrm{C}^*\varphi) \quad \textit{and} \quad [\langle \mathrm{A}, \mathrm{CA}\rangle, a^*(\varphi)] = a(\mathrm{C}\varphi)^*, \tag{3.17}$$

where we recall that $[A, B] = AB - BA$, for any $A, B \in \mathcal{U}$.

Proof: We will give only the proof of the first equation, the other one being proven exactly in the same way. By using the definition of bilinear elements, one has

$$\begin{aligned} [\langle \mathrm{A}, \mathrm{CA}\rangle, a(\varphi)] &= \sum_{i,j\in I} \left\langle \psi_i, \mathrm{C}\psi_j \right\rangle_{\mathfrak{h}} \left[a\left(\psi_i\right)^* a\left(\psi_j\right), a(\varphi) \right] \\ &= \sum_{i,j\in I} \left\langle \psi_i, \mathrm{C}\psi_j \right\rangle_{\mathfrak{h}} \left(a\left(\psi_i\right)^* a\left(\psi_j\right) a(\varphi) - a(\varphi) a\left(\psi_i\right)^* a\left(\psi_j\right) \right). \end{aligned}$$

By the CAR properties given in Equation (3.8)), one has

$$\begin{aligned} a\left(\psi_i\right)^* a\left(\psi_j\right) a(\varphi) &= -\, a\left(\psi_i\right)^* a(\varphi) a\left(\psi_j\right) \\ &= -\, \langle \varphi, \psi_i \rangle_{\mathfrak{h}}\, a(\psi_j) + a(\varphi) a\left(\psi_i\right)^* a\left(\psi_j\right). \end{aligned}$$

This leads to

$$\begin{aligned} [\langle \mathrm{A}, \mathrm{CA}\rangle, a(\varphi)] &= -\sum_{i,j\in I} \left\langle \psi_i, \mathrm{C}\psi_j \right\rangle_{\mathfrak{h}} \left\langle \psi_i, \varphi \right\rangle_{\mathfrak{h}} a(\psi_j) \\ &= -\sum_{j\in I} \left\langle \mathrm{C}^*\varphi, \psi_j \right\rangle_{\mathfrak{h}} a(\psi_j) \\ &= -\, a(\mathrm{C}^*\varphi). \end{aligned}$$

The other equality is proved in the same way. ■

Note from Proposition 3.2.4 that, for $\mathrm{C}_1, \mathrm{C}_2 \in \mathcal{B}(\mathfrak{h})$ whose ranges are finite dimensional,

$$[\langle \mathrm{A}, \mathrm{C}_1\mathrm{A}\rangle, \langle \mathrm{A}, \mathrm{C}_2\mathrm{A}\rangle] = \langle \mathrm{A}, [\mathrm{C}_1, \mathrm{C}_2]\, \mathrm{A}\rangle. \tag{3.18}$$

Moreover, Proposition 3.2.4 yields the following corollary:

Corollary 3.2.5 ("Bogoliubov" property)
For any $C \in \mathcal{B}(\mathfrak{h})$ whose range is finite-dimensional and for any $\varphi \in \mathfrak{h}$, one has

$$\mathrm{e}^{\langle \mathrm{A}, C\mathrm{A}\rangle} a(\varphi) \mathrm{e}^{-\langle \mathrm{A}, C\mathrm{A}\rangle} = a(\mathrm{e}^{-C^*}\varphi) \quad \textit{and} \quad \mathrm{e}^{\langle \mathrm{A}, C\mathrm{A}\rangle} a^*(\varphi) \mathrm{e}^{-\langle \mathrm{A}, C\mathrm{A}\rangle} = a^*(\mathrm{e}^{C}\varphi). \tag{3.19}$$

Proof: We will give only the proof of the first equation, the other one being proven exactly in the same way. Assuming the hypothesis of the corollary, consider the mapping from $\mathbb{R}$ to $\mathcal{U}$ defined by

$$t \mapsto \mathrm{e}^{-t\langle \mathrm{A}, C\mathrm{A}\rangle} a(\mathrm{e}^{-tC^*}\varphi) \mathrm{e}^{t\langle \mathrm{A}, C\mathrm{A}\rangle}.$$

By a direct computation, note that

$$\frac{d}{dt}\left(\mathrm{e}^{-t\langle \mathrm{A}, C\mathrm{A}\rangle} a(\mathrm{e}^{-tC^*}\varphi) \mathrm{e}^{t\langle \mathrm{A}, C\mathrm{A}\rangle}\right) = -\left[\langle \mathrm{A}, C\mathrm{A}\rangle, \mathrm{e}^{-t\langle \mathrm{A}, C\mathrm{A}\rangle} a(\mathrm{e}^{-tC^*}\varphi) \mathrm{e}^{t\langle \mathrm{A}, C\mathrm{A}\rangle}\right] - \mathrm{e}^{-t\langle \mathrm{A}, C\mathrm{A}\rangle} a(C^*\mathrm{e}^{-tC^*}\varphi) \mathrm{e}^{t\langle \mathrm{A}, C\mathrm{A}\rangle}. \tag{3.20}$$

By using Proposition 3.2.4, one has

$$a(C^*\mathrm{e}^{tC^*}\varphi) = -\left[\langle \mathrm{A}, C\mathrm{A}\rangle, a(\mathrm{e}^{-tC^*}\varphi)\right].$$

By using this equality in Equation (3.20), one has that:

$$\frac{d}{dt}\left(\mathrm{e}^{-t\langle \mathrm{A}, C\mathrm{A}\rangle} a(\mathrm{e}^{-tC^*}\varphi) \mathrm{e}^{t\langle \mathrm{A}, C\mathrm{A}\rangle}\right) = 0.$$

In particular, it is constant with respect to $t \in \mathbb{R}$. By taking its value for $t = 0$ and $t = 1$ one concludes that:

$$\mathrm{e}^{-\langle \mathrm{A}, C\mathrm{A}\rangle} a(\mathrm{e}^{-C^*}\varphi) \mathrm{e}^{\langle \mathrm{A}, C\mathrm{A}\rangle} = a(\varphi).$$

The other equality is proven in the same way. ∎

We are now in a position to define the so-called *quasi-free dynamics*.

Definition 3.2.6 (Quasi-free dynamics)
Let h be a self-adjoint operators in $\mathcal{B}(\mathfrak{h})$. We define the strongly continuous group $\{\tau_t\}_{t\in\mathbb{R}}$ of $*$-automorphisms of $\mathcal{U}$ by:

$$\tau_t\left(a(\varphi)\right) = a(\mathrm{e}^{ith}\varphi) \quad \textit{and} \quad \tau_t\left(a^*(\varphi)\right) = a^*(\mathrm{e}^{ith}\varphi), \quad \varphi \in \mathfrak{h}. \tag{3.21}$$

The automorphism satisfying Equation (3.21) is an example of *Bogoliubov* $*$-automorphism. It is directly related with bilinear elements:

Proposition 3.2.7 (*Bogoliubov* $*$-automorphism and bilinear elements)
Let h be a self-adjoint operator in $\mathcal{B}(\mathfrak{h})$ whose range is finite-dimensional. Then, the continuous group $\{\tau_t\}_{t\in\mathbb{R}}$ of Definition 3.2.6 satisfies

$$\tau_t(B) := \mathrm{e}^{it\langle \mathrm{A}, h\mathrm{A}\rangle} B \mathrm{e}^{-it\langle \mathrm{A}, h\mathrm{A}\rangle}, \qquad B \in \mathcal{U}.$$

In particular, the generator of the group $\{\tau_t\}_{t\in\mathbb{R}}$ is the bounded operator δ defined by

$$\delta(B) = i\left[\langle \mathrm{A}, h\mathrm{A}\rangle, B\right], \quad B \in \mathcal{U}. \tag{3.22}$$

Proof: This is a direct consequence of Corollary 3.2.5 and the fact that $\{\tau_t\}_{t\in\mathbb{R}}$ is a family of $*$-automorphisms. ■

Quasi-free dynamics have a good behavior with respect to convergence of bounded Hamiltonian. To see this, we first recall an elementary observation on the exponential function:

Proposition 3.2.8 (Trotter)
Let $(h_n)_{n\in\mathbb{N}} \subseteq \mathcal{B}(\mathfrak{h})$ be a family of bounded, self-adjoint operators converging to $h_\infty \in \mathcal{B}(\mathfrak{h})$ in the strong topology. Then, for any $t \in \mathbb{R}$, $\left(\mathrm{e}^{ith_n}\right)_{n\in\mathbb{N}}$ converges to e^{ith_∞} in the strong topology.

Proof: This statement is standard. For the reader's convenience, we give its proof. It is clear that there exists a constant $D \in \mathbb{R}$ such that

$$\sup_{n\in\mathbb{N}\cup\{\infty\}} \|h_n\|_{\mathcal{B}(\mathfrak{h})} \leq D\,. \tag{3.23}$$

Since, for all $k \in \mathbb{N}$,

$$A^k - B^k = A^{k-1}(A-B) + (A^{k-1} - B^{k-1})B, \quad A, B \in \mathcal{B}(\mathfrak{h}),$$

by a mathematical induction, one can easily show that $(h_n^k)_{n\in\mathbb{N}}$ converges strongly to h_∞^k in $\mathcal{B}(\mathfrak{h})$ for $k \in \mathbb{N}$. Furthermore, by using the triangle inequality, one has, for $\psi \in \mathfrak{h}$,

$$\|\mathrm{e}^{ith_n}\psi - \mathrm{e}^{ith}\psi\|_{\mathfrak{h}} \leq \sum_{k\geq 0} \frac{|t|}{k!}\|h_n^k\psi - h_\infty^k\psi\|_{\mathfrak{h}} \tag{3.24}$$

$$\leq \sum_{k\geq 0} \frac{|t|}{k!}\left(\|h_n^k\psi\|_{\mathfrak{h}} + \|h_\infty^k\psi\|_{\mathfrak{h}}\right). \tag{3.25}$$

By (3.23), one can apply the Lebesgue's dominated convergence theorem in (3.24) to conclude the proof. ■

As a consequence, we obtain the following result:

Proposition 3.2.9 (Infinite-volume quasi-free dynamics)
Let $(h_n)_{n\in\mathbb{N}} \subseteq \mathcal{B}(\mathfrak{h})$ be a family of self-adjoint operators converging to $h_\infty \in \mathcal{B}(\mathfrak{h})$ in the strong topology. For any $n \in \mathbb{N}\cup\{\infty\}$, denote by $\left\{\tau_t^n\right\}_{t\in\mathbb{R}}$ the strongly continuous group of Definition 3.2.6, for $h = h_n$. Then, $\left\{\tau_t^n\right\}_{t\in\mathbb{R}}$ strongly converges, as $n \to \infty$, to $\left\{\tau_t^\infty\right\}_{t\in\mathbb{R}}$.

Proof: For $n \in \mathbb{N}\cup\{\infty\}$, $t \in \mathbb{R}$, τ_t^n is a $*$-automorphism and, in particular, belongs to the unit ball of $\mathcal{B}(\mathfrak{h})$, see (1.10). Therefore, it suffices to consider monomials in $a(\psi)$ and $a^*(\psi)$ for $\psi \in \mathfrak{h}$ to prove the assertion. Since, by Proposition 3.1.5,

$$\|a(\mathrm{e}^{ith_\infty}\psi) - a(\mathrm{e}^{ith_n}\psi)\|_{\mathcal{U}} = \|\mathrm{e}^{ith_\infty}\psi - \mathrm{e}^{ith_n}\psi\|_{\mathfrak{h}},$$

the assertion follows from Proposition 3.2.8. ■

By Proposition 3.2.7, if $(h_n)_{n\in\mathbb{N}} \subseteq \mathcal{B}(\mathfrak{h})$ is a family of self-adjoint operators whose range is finite-dimensional and which converges to h_∞ in the strong topology, then the quasi-free dynamics associated with h_∞ is the strong limit of dynamics generated by bilinear elements associated with h_n. In other words, Definition 3.2.6 is a natural definition to describe the dynamics of non-interacting *fermion* systems.

3.2.4 Quasi-free states

A state ρ is, by definition, a positive linear functional ρ acting on $\mathcal{U}$ such that $\rho(\mathbf{1}) = 1$. Bilinear Hamiltonians are also involved to characterize the so-called *quasi-free states*:

Definition 3.2.10 (Quasi-free states)
A state ρ is defined to be (gauge-invariant) quasi-free if, for all $N_1, N_2 \in \mathbb{N}$ and $\psi_1, \ldots, \psi_{N_1+N_2} \in \mathfrak{h}$,

$$\rho\left(a^*(\psi_1)\cdots a^*(\psi_{N_1})a(\psi_{N_1+N_2})\cdots a(\psi_{N_1+1})\right) = 0 \tag{3.26}$$

if $N_1 \neq N_2$, while in the case $N_1 = N_2 \equiv N$,

$$\rho\left(a^*(\psi_1)\cdots a^*(\psi_N)a(\psi_{2N})\cdots a(\psi_{N+1})\right) = \det\left[\rho\left(a^*(\psi_k)a(\psi_{N+l})\right)\right]_{k,l=1}^{N}. \tag{3.27}$$

See, e.g., [7, Definition 3.1], which refers to a more general notion of quasi-free states. Here, we impose the gauge-invariant property on quasi-free states, which corresponds to Equation (3.26). [7, Definition 3.1, Condition (3.1)] only imposes the quasi–free state to be even, which is a strictly weaker property than being gauge-invariant. As one can see in Definition 3.2.10, *quasi-free states* are particular states in the sense that they are uniquely defined by two-point correlation functions. In fact, for any *quasi-free state* ρ, there exists a unique operator denoted by S_ρ satisfying

$$0 \leq S_\rho \leq \mathbf{1}_\mathfrak{h} \tag{3.28}$$

such that

$$\rho\left(a^*(\varphi_1)a(\varphi_2)\right) = \langle \varphi_2, S_\rho \varphi_1 \rangle, \quad \varphi_1, \varphi_2 \in \mathfrak{h}. \tag{3.29}$$

In the literature, the operator S_ρ is called the *one-particle density matrix* of the system or the *symbol* of the *quasi-free* state ρ. Conversely, any self-adjoint operator that satisfies (3.28) uniquely defines a quasi-free state through Equation (3.29). For more details on *quasi-free states*, see [7, lemma 3.2]. An example, of a *quasi-free state* is given by the so-called tracial state:

Definition 3.2.11 (Tracial state)
The tracial state, denoted by tr*, is the quasi-free state with symbol equal to*

$$S_{\mathrm{tr}} := \frac{1}{2}\mathbf{1}_\mathfrak{h}.$$

As it is mentioned at the beginning of this section, bilinear Hamiltonians are involved to characterize *quasi-free states*:

Lemma 3.2.12 (Quasi-free states)
Let $\beta \in \mathbb{R}^+$ and $h \in \mathcal{B}(\mathfrak{h})$ be a self-adjoint operator whose range is finite-dimensional. Then, the state

$$\rho_h(B) := \frac{\mathrm{tr}\left(B\mathrm{e}^{-\beta\langle \mathrm{A}, h\mathrm{A}\rangle}\right)}{\mathrm{tr}\left(\mathrm{e}^{-\beta\langle \mathrm{A}, h\mathrm{A}\rangle}\right)}, \quad B \in \mathcal{U}, \tag{3.30}$$

is a quasi-free state with symbol

$$S_{\rho_h} = \left(1 + \mathrm{e}^{\beta h}\right)^{-1}.$$

In particular, for any $\varphi, \psi \in \mathfrak{h}$,

$$\rho_h\left(a^*(\varphi)a(\psi)\right) = \left\langle \psi, \left(1 + \mathrm{e}^{\beta h}\right)^{-1}\varphi\right\rangle_{\mathfrak{h}}. \tag{3.31}$$

Proof: Let $\tau := \{\tau_t\}_{t\in\mathbb{R}}$ be the strongly continuous group of $*$-automorphisms of $\mathcal{U}$ given in Definition 3.2.6. By Proposition 3.2.7 and Definition 2.2.1, ρ_h is a (τ, β)-KMS state. Since τ_t can be analytically extended to all $z \in \mathbb{C}$, we have in particular

$$\rho_h\left(B\tau_{i\beta}(C)\right) = \rho_h\left(C\,B\right), \quad B, C \in \mathcal{U}.$$

By using the CAR properties in (3.12) and Definition 3.2.6, we compute that, for any $\varphi, \psi \in \mathfrak{h}$,

$$\rho_h\left(a^*(\varphi)a(\psi)\right) = \rho_h\left(a(\psi)\tau_{i\beta}\left(a^*(\varphi)\right)\right) \tag{3.32}$$

$$= \rho_h\left(a(\psi)a^*(\mathrm{e}^{-\beta h}\varphi)\right) \tag{3.33}$$

$$= \left\langle \psi, \mathrm{e}^{-\beta h}\varphi\right\rangle_{\mathfrak{h}} - \rho_h\left(a^*(\mathrm{e}^{-\beta h}\varphi)a(\psi)\right) \tag{3.34}$$

Since $h \in \mathcal{B}(\mathfrak{h})$ has finite-dimensional range, $\mathfrak{h} = \mathcal{H} \oplus \ker(h)$ with $\mathcal{H}$ being a finite-dimensional subspace. For any $\psi \in \mathfrak{h}$ and $\varphi \in \ker(h)$, it follows that

$$\rho_h\left(a^*(\varphi)a(\psi)\right) = \frac{1}{2}\left\langle \psi, \varphi\right\rangle_{\mathfrak{h}} = \left\langle \psi, S_{\rho_h}\varphi\right\rangle_{\mathfrak{h}}.$$

Now, for any $\psi \in \mathfrak{h}$ and (non-zero) $\varphi \in \mathcal{H}$, we iterate $n \in \mathbb{N}$ times the equation (3.34) to obtain that

$$\rho_h\left(a^*(\varphi)a(\psi)\right) = \left\langle \psi, \left(\mathrm{e}^{-\beta h}\left(1 - \mathrm{e}^{-\beta h} + \mathrm{e}^{-2\beta h} + \ldots + (-1)^n\mathrm{e}^{-n\beta h}\right)\right)\varphi\right\rangle_{\mathfrak{h}} + (-1)^{n+1}\rho_h\left(a^*(\mathrm{e}^{-n\beta h}\varphi)a(\psi)\right). \tag{3.35}$$

Because $\mathcal{H}$ has finite dimension and h is self-adjoint, we deduce that

$$\lim_{n\to\infty}\left\|\mathrm{e}^{-n\beta h}\varphi\right\|_{\mathfrak{h}} = 0, \qquad \varphi \in \mathcal{H}. \tag{3.36}$$

Since

$$S_{\rho_h}|_{\mathcal{H}} = \mathrm{e}^{-\beta h} \sum_{n=0}^{\infty} (-1)^n \mathrm{e}^{-n\beta h}|_{\mathcal{H}}$$

and, for any $n \in \mathbb{N}$,

$$\left| \rho_h \left(a^*(\mathrm{e}^{-n\beta h}\varphi) a(\psi) \right) \right| \leq \left\| \mathrm{e}^{-n\beta h}\varphi \right\|_{\mathfrak{h}} \left\| \psi \right\|_{\mathfrak{h}}$$

we infer from (3.35) and (3.36) that, in the limit $n \to \infty$ and for any $\psi \in \mathfrak{h}$ and (non-zero) $\varphi \in \mathcal{H}$,

$$\rho_h \left(a^*(\varphi) a(\psi) \right) = \left\langle \psi, S_{\rho_h} \varphi \right\rangle_{\mathfrak{h}} .$$

■

By [27, Proposition 5.2.23], note that ρ_h is the unique (τ, β)-KMS state with symbol

$$S_{\rho_h} = \left(1 + \mathrm{e}^{\beta h} \right)^{-1} .$$

Similar to Proposition 3.2.9, we also get the following continuity property of quasi-free states:

Proposition 3.2.13 (Infinite-volume quasi-free state)
Let $(h_n)_{n \in \mathbb{N}} \subseteq \mathcal{B}(\mathfrak{h})$ be a family of self-adjoint operators converging to $h_\infty \in \mathcal{B}(\mathfrak{h})$ in the strong topology. For any $n \in \mathbb{N} \cup \{\infty\}$, denote by ρ_{h_n} the quasi-free state of Definition 3.2.6 with symbol $S_{\rho_{h_n}} = \left(1 + \mathrm{e}^{\beta h_n} \right)^{-1}$. Then, ρ_{h_n} converges, as $n \to \infty$, to ρ_{h_∞}, in the weak* topology, that is, for any $B \in \mathcal{U}$,

$$\lim_{n \to \infty} \rho_{h_n}(B) = \rho_{h_\infty}(B) .$$

Proof: Take all parameters of the proposition. By the second resolvent identity, for any $\beta \in \mathbb{R}^+$ and $n \in \mathbb{N}$,

$$S_{\rho_{h_n}} - S_{\rho_{h_\infty}} = \frac{1}{1 + \mathrm{e}^{\beta h_n}} - \frac{1}{1 + \mathrm{e}^{\beta h_\infty}} = \frac{1}{1 + \mathrm{e}^{\beta h_n}} \left(\mathrm{e}^{\beta h_\infty} - \mathrm{e}^{\beta h_n} \right) \frac{1}{1 + \mathrm{e}^{\beta h_\infty}} . \tag{3.37}$$

Since $(h_n)_{n \in \mathbb{N}} \subseteq \mathcal{B}(\mathfrak{h})$ strongly converges to $h_\infty \in \mathcal{B}(\mathfrak{h})$, one infers from (3.37) and Proposition 3.2.8 that, for any $\psi \in \mathfrak{h}$,

$$\lim_{n \to \infty} \| S_{\rho_{h_n}} \psi - S_{\rho_{h_\infty}} \psi \|_{\mathfrak{h}} = 0.$$

In other words, $S_{\rho_{h_n}}$ strongly converges to $S_{\rho_{h_\infty}}$. Therefore, by (3.29),

$$\lim_{n \to \infty} \rho_{h_n} \left(a^*(\varphi) a(\psi) \right) = \rho_{h_\infty} \left(a^*(\varphi) a(\psi) \right) , \quad \varphi, \psi \in \mathfrak{h}.$$

By the quasi-free state property, see Definition 3.2.10, one obtains the weak* convergence of ρ_{h_n} towards ρ_{h_∞}.

■

Chapter 4

Charge and Heat Transport Properties of Fermions in a Disordered Media

Throughout this thesis, among the works that have been done, we study the classical conductivity theory near the atomic scale, at which quantum effects should dominate. In recent history, such an interest has been motivated by the growing need for smaller electronic components. In 2012, experimental measurements of electric resistance of nanowires in Si doped with phosphorus atoms demonstrate that quantum effects on charge transport almost disappear for nanowires of lengths larger than a few nanometers, even at very low temperature ($4.2K$). We mathematically prove, for non-interacting lattice fermions with disorder, that quantum uncertainty of microscopic electric current density around their (classical) macroscopic values is suppressed, exponentially fast with respect to the volume of the region of the lattice where an external electric field is applied. This is in accordance with the above experimental observation. Furthermore, this result is a continuation of a series of articles recently published, for instance [34, 29], where the authors showed the convergence of the expectation values of microscopic current densities. However, no information about the suppression of quantum uncertainty was obtained in the macroscopic limit within these papers. Another problem that has been studied within the pre-doctoral period is a derivation of the celebrated heat equation by using the principles of quantum mechanics. We give some preliminary results about this, which can be taken as a first step in order to get the well-known (classical) equation introduced by J. Fourier in 1807.

4.1 Hilbert space formulation of one lattice fermion in disordered media

The host material: For conducting spinless *fermions*, let us consider a cubic crystal represented by the d–dimensional cubic lattice $\mathbb{Z}^d$ ($d \in \mathbb{N}$). Below, $\mathcal{P}_f(\mathbb{Z}^d) \subset 2^{\mathbb{Z}^d}$ is the set of all non-empty *finite* subsets of $\mathbb{Z}^d$. Further,

$$\mathbb{D} := \{z \in \mathbb{C} : |z| \leq 1\} \quad \text{and} \quad \mathfrak{b} := \left\{\{x, x'\} \subset \mathbb{Z}^d : |x - x'| = 1\right\}$$

is the set of (non–oriented) edges of the cubic lattice $\mathbb{Z}^d$.

Disordered Media: Disorder in the crystal is modeled by a random variable taking values in the measurable space $(\Omega, \mathfrak{A}_\Omega)$, with distribution $\mathfrak{a}_\Omega$:

Ω : Elements of Ω are pairs $\omega = (\omega_1, \omega_2) \in \Omega$, where ω_1 is a function on lattice sites with values in the interval $[-1,1]$ and ω_2 is a function on edges with values in the complex closed unit disc $\mathbb{D}$. In other words,

$$\Omega := [-1,1]^{\mathbb{Z}^d} \times \mathbb{D}^{\mathfrak{b}}.$$

$\mathfrak{A}_\Omega$: Let $\Omega_x^{(1)}$, $x \in \mathbb{Z}^d$, be an arbitrary element of the Borel σ–algebra $\mathfrak{A}_x^{(1)}$ of the interval $[-1,1]$ with respect to the usual metric topology. Define

$$\mathfrak{A}_{[-1,1]^{\mathbb{Z}^d}} := \bigotimes_{x\in\mathbb{Z}^d} \mathfrak{A}_x^{(1)}, \tag{4.1}$$

i.e., $\mathfrak{A}_{[-1,1]^{\mathbb{Z}^d}}$ is the σ–algebra generated by the cylinder sets $\prod_{x\in\mathbb{Z}^d} \Omega_x^{(1)}$, where $\Omega_x^{(1)} = [-1,1]$ for all but finitely many $x \in \mathbb{Z}^d$. In the same way, let

$$\mathfrak{A}_{\mathbb{D}^{\mathfrak{b}}} := \bigotimes_{\mathbf{x}\in\mathfrak{b}} \mathfrak{A}_{\mathbf{x}}^{(2)} ,$$

where $\mathfrak{A}_{\mathbf{x}}^{(2)}$, $\mathbf{x} \in \mathfrak{b}$, is the Borel σ–algebra of the complex closed unit disc $\mathbb{D}$ with respect to the usual metric topology. Then

$$\mathfrak{A}_\Omega := \mathfrak{A}_{[-1,1]^{\mathbb{Z}^d}} \otimes \mathfrak{A}_{\mathbb{D}^{\mathfrak{b}}} .$$

$\mathfrak{a}_\Omega$: The distribution $\mathfrak{a}_\Omega$ is an arbitrary *ergodic* probability measure on the measurable space $(\Omega, \mathfrak{A}_\Omega)$. I.e., it is invariant under the action

$$(\omega_1, \omega_2) \longmapsto \chi_x^{(\Omega)}(\omega_1, \omega_2) := \left(\chi_x^{(\mathbb{Z}^d)}(\omega_1), \chi_x^{(\mathfrak{b})}(\omega_2)\right) , \qquad x \in \mathbb{Z}^d , \tag{4.2}$$

of the group $(\mathbb{Z}^d, +)$ of translations on Ω and $\mathfrak{a}_\Omega(\mathcal{X}) \in \{0,1\}$ whenever $\mathcal{X} \in \mathfrak{A}_\Omega$ satisfies $\chi_x^{(\Omega)}(\mathcal{X}) = \mathcal{X}$ for all $x \in \mathbb{Z}^d$. Here, for any $\omega = (\omega_1, \omega_2) \in \Omega$, $x \in \mathbb{Z}^d$ and $y, y' \in \mathbb{Z}^d$ with $|y - y'| = 1$,

$$\chi_x^{(\mathbb{Z}^d)}(\omega_1)(y) := \omega_1(y+x), \ \chi_x^{(\mathfrak{b})}(\omega_2)(\{y,y'\}) := \omega_2(\{y+x, y'+x\}) . \tag{4.3}$$

As is usual, $\mathbb{E}[\cdot]$ denotes the expectation value associated with $\mathfrak{a}_\Omega$.

The one-particle Hilbert space: From now on and in all this chapter, the one-particle Hilbert space is $\mathfrak{h} := \ell^2(\mathbb{Z}^d; \mathbb{C})$, which is defined by

$$\ell^2(\mathbb{Z}^d; \mathbb{C}) \equiv \ell^2(\mathbb{Z}^d) := \left\{ \psi : \mathbb{Z}^d \mapsto \mathbb{C} : \sum_{x \in \mathbb{Z}^d} |\psi(x)|^2 < \infty \right\}.$$

Its canonical orthonormal basis is denoted by $\{\mathfrak{e}_x\}_{x \in \mathbb{Z}^d}$, defined by

$$\mathfrak{e}_x(y) := \delta_{x,y} \quad \text{for all } x, y \in \mathbb{Z}^d. \tag{4.4}$$

The one-particle Hamiltonian: To any $\omega \in \Omega$ and strength $\vartheta \in \mathbb{R}_0^+$ of hopping disorder, we associate a self–adjoint operator $\Delta_{\omega,\vartheta} \in \mathcal{B}(\mathfrak{h})$ describing the hoppings of a single particle in the lattice:

$$[\Delta_{\omega,\vartheta}(\psi)](x) := 2d\psi(x) - \sum_{j=1}^{d} \Big((1 + \vartheta \overline{\omega_2(\{x, x - e_j\})})\, \psi(x - e_j) \tag{4.5}$$

$$+ \psi(x + e_j)(1 + \vartheta \omega_2(\{x, x + e_j\})) \Big) \tag{4.6}$$

for any $x \in \mathbb{Z}^d$ and $\psi \in \mathfrak{h} := \ell^2(\mathbb{Z}^d)$, with $\{e_k\}_{k=1}^d$ being the canonical orthonormal basis of the Euclidian space $\mathbb{R}^d$. In the case of vanishing hopping disorder $\vartheta = 0$, (up to a minus sign) $\Delta_{\omega,0} \equiv \Delta_{\mathrm{d}}$ is the usual d–dimensional discrete Laplacian. Since the hopping amplitudes are complex–valued (ω_2 takes values in $\mathbb{D}$), note additionally that random electromagnetic potentials can be implemented in our model. Then, the random tight-binding model is the one-particle Hamiltonian defined by

$$h^{(\omega)} := \Delta_{\omega,\vartheta} + \lambda\omega_1 , \qquad \omega = (\omega_1, \omega_2) \in \Omega,\ \lambda, \vartheta \in \mathbb{R}_0^+, \tag{4.7}$$

where the function $\omega_1 : \mathbb{Z}^d \to [-1, 1]$ is identified with the corresponding (self-adjoint) multiplication operator. We use this operator to define a (infinite volume) dynamics, by the unitary group $\{\mathrm{e}^{ith^{(\omega)}}\}_{t \in \mathbb{R}}$, in the one–particle Hilbert space $\mathfrak{h}$. Note that the tight-binding Anderson model corresponds to the special case $\vartheta = 0$.

Spacial restriction: Within the technical proofs, instead of working on the infinite lattice, we consider various spatial restrictions and take the thermodynamic limit. For this issue, consider the finite box $\Lambda_\ell \in \mathcal{P}_f(\mathbb{Z}^d)$ defined by

$$\Lambda_\ell := \{(x_1, \ldots, x_d) \in \mathbb{Z}^d : |x_1|, \ldots, |x_d| \leq \ell\} \in \mathcal{P}_f(\mathbb{Z}^d), \qquad \ell \in \mathbb{R}_0^+. \tag{4.8}$$

For any $\Lambda \in \mathcal{P}_f(\mathbb{Z}^d)$, let P_Λ be the orthogonal projection defined on $\mathfrak{h} := \ell^2(\mathbb{Z}^d)$ by

$$[P_\Lambda(\varphi)](x) := \begin{cases} \varphi(x) & , \quad \text{if } x \in \Lambda. \\ 0 & , \quad \text{else.} \end{cases} \tag{4.9}$$

Then, the one-particle Hamiltonian within Λ_ℓ is equal to

$$h_{\Lambda_\ell} := P_{\Lambda_\ell} h^{(\omega)} P_{\Lambda_\ell}, \tag{4.10}$$

leading to the unitary group $\{e^{ith_{\Lambda_\ell}}\}_{t\in\mathbb{R}}$. Now let us introduce the following (standard) result:

Proposition 4.1.1 (Strong convergence of local Hamiltonians)
The family $(h_{\Lambda_\ell})_{\ell\in\mathbb{R}_0^+} \subset \mathcal{B}(\mathfrak{h})$ *strongly converges to* $h^{(\omega)} \in \mathcal{B}(\mathfrak{h})$.

Proof: This proof is straightforward. We give it for completenes. Since $h^{(\omega)} \in \mathcal{B}(\mathfrak{h})$, we deduced from the triangle inequality that, for any $\psi \in \mathfrak{h}$,

$$\begin{aligned} \|h^{(\omega)}(\psi) - h_{\Lambda_\ell}(\psi)\|_{\mathfrak{h}} \leq \|h^{(\omega)}(\psi) - P_{\Lambda_\ell} h^{(\omega)}(\psi))\|_{\mathfrak{h}} \\ + \|h^{(\omega)}\|_{\mathcal{B}(\mathfrak{h})} \|\psi - P_{\Lambda_\ell}(\psi)\|_{\mathfrak{h}} \end{aligned}$$

Therefore, it suffices to prove that

$$\lim_{\ell\to\infty} P_{\Lambda_\ell}\psi = \psi, \quad \psi \in \mathfrak{h}.$$

to get the assertion. The last equality is obvious: Since $\{\mathfrak{e}_x\}_{x\in\mathbb{Z}^d}$ is the canonical orthonormal basis of the Hilbert space $\mathfrak{h} := \ell^2(\mathbb{Z}^d;\mathbb{C})$, as defined by (4.4), it is completly standard that any $\psi \in \mathfrak{h}$ can be written[1] as

$$\psi = \sum_{x\in\mathbb{Z}^d} \langle \psi, \mathfrak{e}_x \rangle_{\mathfrak{h}} \, \mathfrak{e}_x$$

with

$$\left\|\psi\right\|_{\mathfrak{h}}^2 = \sum_{x\in\mathbb{Z}^d} \left|\langle \psi, \mathfrak{e}_x \rangle_{\mathfrak{h}}\right|^2 < \infty. \tag{4.11}$$

Therefore, by (4.9) and the triangle inequality, for any $\Lambda \in \mathcal{P}_f(\mathbb{Z}^d)$,

$$\|P_{\Lambda_\ell}\psi - \psi\|_{\mathfrak{h}} \leq \sum_{x\in\mathbb{Z}^d\backslash\Lambda} \left|\langle \psi, \mathfrak{e}_x \rangle_{\mathfrak{h}}\right|^2. \tag{4.12}$$

By (4.11)-(4.12), it obviously follows that

$$\lim_{\ell\to\infty} \|P_{\Lambda_\ell}\psi - \psi\|_{\mathfrak{h}} = 0.$$

This concludes the proof. ■

[1]The equality means of course that the sum on the right-hand side converges to ψ in $\mathfrak{h}$.

Combes-Thomas estimate: By the Combes-Thomas estimate (Chapter 7, Section 7.7),

$$\left|\left\langle \mathfrak{e}_x, \mathrm{e}^{ith^{(\omega)}} \mathfrak{e}_y \right\rangle_{\mathfrak{h}}\right| \leq 36\mathrm{e}^{|t\eta|-2\mu_\eta|x-y|} \tag{4.13}$$

for any $\eta, \mu \in \mathbb{R}^+$, $x, y \in \mathbb{Z}^d$ and $\lambda, \vartheta \in \mathbb{R}_0^+$, where

$$\mu_\eta := \mu \min\left\{\frac{1}{2}, \frac{\eta}{8d\,(1+\vartheta)\,\mathrm{e}^{\mu}}\right\}. \tag{4.14}$$

See Corollary 7.7.2, by observing that the parameter $\mathbf{S}$ defined by (7.78) is bounded in this case by $\mathbf{S}(h_{\mathcal{Z}}^{(\omega)}, \mu) \leq 2d(1+\vartheta)\mathrm{e}^{\mu}$.

4.2 Algebraic Setting

We use the algebraic formulation for lattice fermion systems, as explained in the previous chapter.

CAR C^*-algebra: The CAR C^*-algebra of the lattice is

$$\mathcal{U} \equiv \mathcal{U}_{\mathbb{Z}^d} \equiv \mathrm{CAR}\left(\ell^2(\mathbb{Z}^d;\mathbb{C})\right),$$

as defined by Definition 3.2.1 with the one-particle Hilbert space $\mathfrak{h} := \ell^2(\mathbb{Z}^d;\mathbb{C})$. Recall in particular that the elements $\{a(\psi)\}_{\psi\in\mathfrak{h}}$ satisfies the canonical anticommutation relations (3.12), that are, for all $\psi, \varphi \in \mathfrak{h}$,

$$a(\psi)a(\varphi) = -a(\varphi)a(\psi), \quad a(\psi)a(\varphi)^* + a(\varphi)^*a(\psi) = \langle\psi,\varphi\rangle_{\mathfrak{h}}\,\mathbf{1}. \tag{4.15}$$

For all $\Lambda \subseteq \mathbb{Z}^d$, note that

$$\mathfrak{h}_\Lambda := \ell^2(\Lambda;\mathbb{C}) \subseteq \mathfrak{h} \equiv \mathfrak{h}_{\mathbb{Z}^d}$$

and $\mathcal{U}_\Lambda \subseteq \mathcal{U}$ is, by definition, the unital C^*-subalgebra generated by the unit $\mathbf{1}$ and the family $\{a(\psi)\}_{\psi\in\mathfrak{h}_\Lambda}$. By separability of $\ell^2(\Lambda;\mathbb{C})$ for any $\Lambda \subseteq \mathbb{Z}^d$, $\mathcal{U}_\Lambda$ is of course always separable and if $\Lambda \in \mathcal{P}_f(\mathbb{Z}^d)$ then $\mathcal{U}_\Lambda$ is finite-dimensional, by [27, Theorem 5.2.5 (2)-(3)]. A *dense* normed $*$-subalgebra of the CAR C^*-algebra $\mathcal{U}$ is given by

$$\mathcal{U}_0 \doteq \bigcup_{\Lambda\in\mathcal{P}_f(\mathbb{Z}^d)} \mathcal{U}_\Lambda\,, \tag{4.16}$$

see [27, Example 5.2.7]. The elements of $\mathcal{U}_0$ are called the local elements of $\mathcal{U}$.

Bilinear Hamiltonians: By Proposition 3.1.7, for any finite subset $\Lambda \in \mathcal{P}_f(\mathbb{Z}^d)$, the second quantization of the restriction to $\mathfrak{h}_\Lambda$ of the one-particle Hamiltonian $h^{(\omega)}$ defined by (4.7) for all $\omega = (\omega_1, \omega_2) \in \Omega,\ \lambda, \vartheta \in \mathbb{R}_0^+$, leads to the bilinear hamiltonian

$$H_\Lambda^{(\omega)} := \sum_{x,y\in\Lambda} \left\langle \mathfrak{e}_x, h^{(\omega)}\left(\mathfrak{e}_y\right)\right\rangle_{\mathfrak{h}} a^*(\mathfrak{e}_x)a(\mathfrak{e}_y)\ . \tag{4.17}$$

This bilinear Hamiltonian is given only as pedagogical exemple of local energy obervables of the system under consideration, but it is not really used in the sequel.

The (autonomous) dynamical system: For all $\omega \in \Omega$ and $\lambda, \vartheta \in \mathbb{R}_0^+$, the dynamics on the CAR C^* –algebra $\mathcal{U}$ is defined by a strongly continuous group $\tau^{(\omega)} := \{\tau_t^{(\omega)}\}_{t\in\mathbb{R}}$ of (Bogoliubov) ∗–automorphisms of $\mathcal{U}$ satisfying

$$\tau_t^{(\omega)}(a(\psi)) = a(\mathrm{e}^{ith^{(\omega)}}\psi)\ , \qquad t \in \mathbb{R}\ ,\ \psi \in \mathfrak{h}. \tag{4.18}$$

See Definition 3.2.6, Proposition 3.2.9 as well as [27, Theorem 5.2.5] for more details on Bogoliubov automorphisms. Let $\delta^{(\omega)}(\cdot)$ whose domain is dense in $\mathcal{U}$ be the generator of $\tau^{(\omega)} := \{\tau_t^{(\omega)}\}_{t\in\mathbb{R}}$. Similarly, for any $\Lambda_\ell \in \mathcal{P}_f(\mathbb{Z}^d)$, we define the strongly continuous group $\tau^{(\omega,\Lambda_\ell)}$ by replacing $h^{(\omega)}$ in (4.18) with $h_{\Lambda_\ell}^{(\omega)}$ (see (4.10)). Since, by Proposition 4.1.1, the operators h_{Λ_ℓ} strongly converges to $h^{(\omega)}$, as $\ell \to \infty$, we infer from Proposition 3.2.9 that, for any $t \in \mathbb{R}$, $\tau_t^{(\omega,\{\Lambda_\ell\})}$ strongly converges to $\tau_t^{(\omega)} \equiv \tau_t^{(\omega,\{\mathbb{Z}^d\})}$, as $\ell \to \infty$.

The states on the C^*-algebra: For any realization $\omega \in \Omega$ and disorder strengths $\lambda, \vartheta \in \mathbb{R}_0^+$, the thermal equilibrium state of the system at inverse temperature $\beta \in \mathbb{R}^+$ is, by definition, the unique $(\tau^{(\omega)}, \beta)$-KMS state $\varrho^{(\omega)}$, see Definition 2.2.1 as well as [27, Example 5.3.2.] or [51, Theorem 5.9]. It is well–known that such a state is stationary with respect to the dynamics $\tau^{(\omega)}$, that is,

$$\varrho^{(\omega)} \circ \tau_t^{(\omega)} = \varrho^{(\omega)}\ , \qquad \omega \in \Omega,\ t \in \mathbb{R}. \tag{4.19}$$

See Equation (2.2) and Theorem 2.2.1. Recall that the state $\varrho^{(\omega)}$ is gauge–invariant and quasi-free, see Definition 3.2.10. It satisfies

$$\varrho^{(\omega)}(a^*(\varphi)\, a(\psi)) = \left\langle \psi, \frac{1}{1+\mathrm{e}^{\beta h^{(\omega)}}}\varphi \right\rangle_{\mathfrak{h}}, \qquad \varphi, \psi \in \mathfrak{h}, \tag{4.20}$$

see Equation (3.31). For $\beta = 0$, one gets the tracial state (or chaotic state), denoted by tr, see Definition 3.2.11. Similarly, for any $\Lambda_\ell \in \mathcal{P}_f(\mathbb{Z}^d)$, we define the quasi-free state $\varrho_{\Lambda_\ell}^{(\omega)}$ by replacing $h^{(\omega)}$ in Equation (4.20) with $h_{\Lambda_\ell}^{(\omega)}$ (see Equation (4.10)). In the thermodynamic limit (large ℓ), we deduce from Propositions 3.2.13 and 4.1.1 that $\varrho_{\{\Lambda_\ell\}}^{(\omega)}$ converges in the weak* topology to $\varrho^{(\omega)} \equiv \varrho_{\{\mathbb{Z}^d\}}^{(\omega)}$.

4.3 Charge transport and heat transport properties

In this section, we start by a setup of the mathematical framework in order to study the heat transport properties from one hand and also the current conductivity properties from the other hand. Our starting points are the results proven by J.B. Bru, W. de Siqueira Pedra and C. Hertling within their papers on Ohm's law, see for instance [33] for the non-interacting case and [29, 30] for the interacting case. We summary the results in a concise way and refers to the corresponding papers for more details.

4.3.1 The electromagnetic potential

Electromagnetic fields induce charge transports. Similar to [33], an electromagnetic potential is applied within a cubic box Λ_ℓ, for $\ell > 0$. Mathematically speaking, it corresponds to a smooth function

$$\mathbf{A} \in \mathbf{C}_0^\infty = \bigcup_{\ell \in \mathbb{R}^+} C_0^\infty(\mathbb{R} \times [-\ell, \ell]^d ; (\mathbb{R}^d)^*) .$$

Recall that $C_0^\infty(\mathbb{R};\mathbb{R})$ is the set of smooth compaclty supported functions from $\mathbb{R}$ to itself. The electric field resulting from this electromagnetic potential is defined by

$$E_{\mathbf{A}}(t,x) := -\partial_t \mathbf{A}(t,x) , \quad t \in \mathbb{R},\ x \in \mathbb{R}^d . \tag{4.21}$$

As an example, picking any normalized (with respect to the usual Euclidian norm) vector $\overrightarrow{w} \in \mathbb{R}^d$, one can consider $\mathbf{A}_\ell$ such that the electric field is given by $E_{\mathbf{A}_\ell}(t,x)\overrightarrow{w}$ at time $t \in \mathbb{R}$, for all $x \in [-\ell,\ell]^d$, and $(0,0,...,0)$, for $t \in \mathbb{R}$ and $x \notin [-\ell,\ell]^d$. We also define the integrated electric field between $y \in \mathbb{Z}^d$ and $x \in \mathbb{Z}^d$ at time $t \in \mathbb{R}$ by

$$\mathbf{E}_t^{\mathbf{A}}(x,y) := \int_0^1 [E_{\mathbf{A}}(t, \alpha y + (1-\alpha)x)]\,(y-x)\mathrm{d}\alpha . \tag{4.22}$$

In the linear response theory, one can rescale the strength of the electromagnetic potential by a real parameter η and study the linear behavior of current densities when $\eta \to 0$. As explained in [34, Section 4.1], in presence of an electromagnetic potential $\mathbf{A} \in C_0^\infty$, one has a time-dependent self-adjoint magnetic Laplacian

$$\Delta_{\omega,\vartheta}^{(\mathbf{A})} \equiv \Delta_{\omega,\vartheta}^{(\mathbf{A}(t,\cdot))} \in \mathcal{B}(\mathfrak{h})$$

defined, for $t \in \mathbb{R}$ and $x, y \in \mathbb{Z}^d$, by

$$\langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}^{(\mathbf{A})} \mathfrak{e}_y \rangle_{\mathfrak{h}} = \exp\left(i \int_0^1 [\mathbf{A}(t, \alpha y + (1-\alpha)x)](y-x) d\alpha \right) \langle \mathfrak{e}_x, \Delta_{\omega,\vartheta} \mathfrak{e}_y \rangle_{\mathfrak{h}}.$$

This yields a time-dependent Hamiltonian defined by

$$\Delta_{\omega,\vartheta}^{(\mathbf{A})} + \lambda\omega_1, \quad t \in \mathbb{R}.$$

This corresponds to a (time-dependent) local energy observable given by

$$H_\Lambda^{(\omega)} + W_t^{(\mathbf{A})} \in \mathcal{U}$$

for any $\Lambda \in \mathcal{P}_f(\mathbb{Z}^d)$, with $H_\Lambda^{(\omega)}$ defined by (4.17) and where

$$W_t^{(\mathbf{A})} := \sum_{x,y\in\Lambda_\ell} \langle \mathfrak{e}_x, (\Delta_{\omega,\vartheta}^{(\mathbf{A})} - \Delta_{\omega,\vartheta})\mathfrak{e}_y\rangle_{\mathfrak{h}} a^*(\mathfrak{e}_x)a(\mathfrak{e}_y) \tag{4.23}$$

is the electromagnetic *potential* energy observable. See also [34, Section 4]. Therefore, one has a perturbed dynamics defined by the random two-parameter family $\{U_{t,s}^{(\omega,\mathbf{A})}\}_{t\geq s}$ of unitary operators on $\mathfrak{h}$. This is the unique solution of the non-autonomous evolution equation

$$\partial_t U_{t,s}^{(\omega,\mathbf{A})} = -i\left(\Delta_{\omega,\vartheta}^{(\mathbf{A})}|_{t=s} + \lambda\omega_1\right) U_{t,s}^{(\omega,\mathbf{A})}, \quad U_{s,s}^{(\omega,\mathbf{A})} := \mathbf{1}_{\mathfrak{h}},$$

for any $\omega \in \Omega$, $\lambda, \vartheta \in \mathbb{R}_0^+$ and $\mathbf{A} \in C_0^\infty$. In presence of electromagnetic potentials $\mathbf{A} \in C_0^\infty$, the perturbed dynamics on $\mathcal{U}$ is on-autonomous and can be written by using the unique strongly continuous two-parameters group $\{\tau_{t,s}^{(\omega,\mathbf{A})}\}_{t,s\in\mathbb{R}}$ of (Bogoliubov) automorphisms (well-) defined by

$$\tau_{t,s}^{(\omega,\mathbf{A})}(a(\psi)) := \tau_{t,s}^{(\omega,\mathbf{A})}(a(\psi)) = a((U_{t,s}^{(\omega,\mathbf{A})})^*\psi), \qquad t,s \in \mathbb{R}, t\geq s\ ,\ \psi \in \mathfrak{h}. \tag{4.24}$$

See [27, Theorem 5.2.5]. Compare with Definition 3.2.6 in the autonomous situation. $\{\tau_{t,s}^{(\omega,\mathbf{A})}\}_{s,t\in\mathbb{R}}$ is a strongly continuous two-parameters family of $*$-automorphisms of $\mathcal{U}$ satisfying

$$\forall s,t \in \mathbb{R}: \qquad \partial_t \tau_{t,s}^{(\omega,\mathbf{A})} = \tau_{t,s}^{(\omega,\mathbf{A})} \circ \delta_t^{(\omega,\mathbf{A})}\ , \qquad \tau_{s,s}^{(\omega,\mathbf{A})} = \mathbf{1}_{\mathcal{U}}\ , \tag{4.25}$$

with

$$\delta_t^{(\omega,\mathbf{A})}(\cdot) := \delta^{(\omega)}(\cdot) + i\left[W_t^{(\mathbf{A})}, \cdot\right]$$

and $\delta^{(\omega)}$ being the infinitesimal generator of the (Bogoliubov) group $\tau^{(\omega)} := \{\tau_t^{(\omega)}\}_{t\in\mathbb{R}}$ of automorphisms defined in the same way by replacing $\Delta_{\omega,\vartheta}^{(\mathbf{A})}$ with $\Delta_{\omega,\vartheta}$ in (4.24), see Equation (4.18). For more details on the perturbed dynamics, see [35, Section 5.2]. Note that the electromagnetic potential is switched on at time $t = 0$, i.e., $\mathbf{A}(t,\cdot) \equiv 0$ for all $t \leq 0$. This refers to the concept of cyclic process, see Definition 2.1.2 in Chapter 2. In the same way as in Equation (2.1), the time evolution of the state of the system is given by:

$$\varrho_t^{(\omega,\lambda,\mathbf{A})} := \begin{cases} \varrho^{(\omega)} & , \qquad t \leq 0\ , \\ \varrho^{(\omega)} \circ \tau_{t,0}^{(\omega,\mathbf{A})} & , \qquad t \geq 0\ . \end{cases} \tag{4.26}$$

4.3.2 Current linear response to electromagnetic fields

As it has already been mentioned, in the context of this work, one deals with non-interacting fermions, i.e,, the state $\varrho^{(\omega)}$ is quasi-free and the observables we consider here are some *2-degrees* polynomial in the annihilation and creation operators. We rely on the algebraic formulation of quantum mechanics, as developed is Chapter 3. Nevertheless, one can formulate the problem in terms of one-particle Hilbert space $\mathfrak{h}$. Indeed, a huge part of the estimates within the technical proofs during the thesis is obtained in the one-particle formulation. In 2007, A. Klein, O. Lenoble and P. Müller published article on conductivity theory and the Anderson model, avoiding completely the algebraic formulation, see [13]. For the sake of clarity and also to compare the object we study within this thesis, we will recall the current formulation in terms of the one-particle Hilbert space, similar to [13]. Recall that a quasi-free state is uniquely characterized by a positive bounded operator $S^{(\omega)}$ on $\mathfrak{h}$, called *symbol*, or *one-particle density matrix*, satisfying

$$0 \leq S^{(\omega)} \leq \mathbf{1}_{\mathfrak{h}}.$$

In our context, as it is said in Equation (4.20), the *symbol* of $\varrho^{(\omega)}$ is defined by

$$S^{(\omega)} := \frac{1}{1 + \mathrm{e}^{\beta(\Delta_{\omega,\vartheta} + \lambda\omega_1)}} \in \mathcal{B}(\mathfrak{h}).$$

Under a perturbation induces by an electromagnetic field, the time-evolving state defined in Equation (4.26) is again *quasi-free* for all times. Its *symbol* is denoted by

$$S_{t,s}^{(\omega,\mathbf{A})} := U_{t,s}^{(\omega,\mathbf{A})} S^{(\omega)} (U_{t,s}^{(\omega,\mathbf{A})})^*.$$

It satisfies the following equality

$$\varrho_t^{(\omega,\mathbf{A})} \left(a^*(\psi) a(\varphi) \right) = \left\langle \varphi, U_{t,s}^{(\omega,\mathbf{A})} S^{(\omega)} (U_{t,s}^{(\omega,\mathbf{A})})^* \psi \right\rangle_{\mathfrak{h}}, \quad \psi, \varphi \in \mathfrak{h}.$$

Since, $(U_{t,s}^{(\omega,\mathbf{A})})^* = U_{s,t}^{(\omega,\mathbf{A})}$ for $t, s \in \mathbb{R}$, the *symbol* of the time-evolving quasi-free state is a solution of the Liouville equation, for $t \geq 0$,

$$\partial_t S_{t,s}^{(\omega,\mathbf{A})} = i \left[\left(\Delta_{\omega,\vartheta}^{(\mathbf{A})} + \lambda\omega_1 \right), S_{t,s}^{(\omega,\mathbf{A})} \right], \quad S_{s,s}^{(\omega,\mathbf{A})} := S^{(\omega)}. \tag{4.27}$$

See also [13, Equation (2.5)]. Now we introduce the algebraic formulation of quantum mechanis which follows the works of J.B. Bru, W. de Siqueira Pedra and C. Hertling. See for instance [34, 29], where they proved the convergence of the expectation values of microscopic current densities in the thermodynamic limit. By using standard tools in probability theory (Large Deviation theory), we sharpen this result by giving a rate of convergence, showing an exponential suppression of quantum uncertainty around the macroscopic (classical) current densities in the thermodynamic limit.

Algebraic current formulation

Currents: Fix $\omega \in \Omega$ and $\vartheta \in \mathbb{R}_0^+$. For any oriented edge $(x, y) \in \left(\mathbb{Z}^d\right)^2$, we define the paramagnetic current observable

$$I_{(x,y)}^{(\omega)} := -2\Im\mathrm{m} \left(\langle \mathfrak{e}_x, \Delta_{\omega,\vartheta} \mathfrak{e}_y \rangle_{\mathfrak{h}} a(\mathfrak{e}_x)^* a(\mathfrak{e}_y) \right). \tag{4.28}$$

The diamagnetic current *observable* is defined by

$$\tilde{I}^{(\omega)}_{(x,y)} = -2\mathfrak{Im}\left(\left(\mathrm{e}^{i\int_0^1[\mathbf{A}(t,\alpha y+(1-\alpha)x)](y-x)d\alpha}-1\right)\langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}} a(\mathfrak{e}_x)^* a(\mathfrak{e}_y)\right). \tag{4.29}$$

Observe that the total current is given by

$$I^{(\omega)}_{(x,y)} + \tilde{I}^{(\omega)}_{(x,y)} = -2\mathfrak{Im}\left(\langle \mathfrak{e}_x, \Delta^{(\mathbf{A})}_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}} a^*(\mathfrak{e}_x)a(\mathfrak{e}_x)\right) =: \mathbf{I}^{(\omega,\mathbf{A})}_{(x,y)} \tag{4.30}$$

It is seen as a current because it satisfies a discrete continuity equation. Indeed, by (4.24) and as it is explained in [30, Section 3.2], in the case of free *fermions* (without interaction),

$$\partial_t\left(\tau^{(\omega)}_{t,s}(a^*(\mathfrak{e}_x)a(\mathfrak{e}_x))\right) = \sum_{y\in\mathbb{Z}^d,|x-y|=1} \tau^{(\omega)}_{t,s}\left(\mathbf{I}^{(\omega,\eta\mathbf{A})}_{x,y}\right).$$

At this point, in order to keep the connection with the one-particle Hilbert space formulation (such as in [13]), let us give the link between the current algebraic formulation and the Hilbert space current formulation. We first introduce some notations. For $\ell > 0$, recall that P_{Λ_ℓ} is the orthogonal projector within the (finite) box Λ_ℓ defined in (4.9). For a positive real number η, we define a (space and strength)-rescaled electromagnetic potential $\eta\mathbf{A}_\ell$ defined as follows: For any $\ell \in \mathbb{R}^+$ and $\mathbf{A} \in C_0^\infty(\mathbb{R}\times[-1;1]^d;\mathbb{R}^d)$, we consider the space-rescaled vector potential

$$\mathbf{A}_\ell(t,x) := \mathbf{A}(t,\ell^{-1}x), \quad t\in\mathbb{R},\ x\in\mathbb{R}^d. \tag{4.31}$$

Denote by $\{e_k\}_{k=1}^d$ the canonical orthonormal basis of the Euclidian space $\mathbb{R}^d$. Note that, by Equation (4.30), the total current density within a box Λ_ℓ in the direction e_k, $k\in\{1,...,d\}$, under an electromagnetic field, is the second quantization of the operator defined by

$$\mathcal{J}^{(\omega)}_\ell := -\frac{2}{|\Lambda_\ell|}\sum_{x\in\Lambda_\ell}\mathfrak{Im}\left\{\left\langle \mathfrak{e}_{x+e_k}, \Delta^{(\eta\mathbf{A}_\ell)}_{\omega,\vartheta}\mathfrak{e}_x\right\rangle_{\mathfrak{h}} P_{\{x+e_k\}}s_{e_k}P_{\{x\}}\right\}, \quad \ell\in\mathbb{R}^+, \tag{4.32}$$

where for any $x\in\mathbb{Z}^d$, the shift operator $s_x\in\mathcal{B}(\mathfrak{h})$ is defined by

$$(s_x\psi)(y) := \psi(x+y), \qquad y\in\mathbb{Z}^d.$$

Note that $s_x^* = s_{-x} = s_x^{-1}$ for any $x\in\mathbb{Z}^d$. See also Equation (7.5), for the definition of the shift operator. Indeed, by using the process of second quantization described in Section 3.5, on obtains that

$$\frac{1}{|\Lambda_\ell|}\sum_{x\in\Lambda_\ell}\mathbf{I}^{(\omega,\eta\mathbf{A}_\ell)}_{(x+e_k,x)} = \left\langle \mathrm{A}, \mathcal{J}^{(\omega)}_\ell \mathrm{A}\right\rangle.$$

The one-particle operator $\mathcal{J}^{(\omega)}_\ell$ corresponds to the commonly current observable in the one-particle Hilbert space which is used for instance in [13]. Indeed, following [13, Section 3], for any $k\in\{1,...,d\}$, let X_k be the (unbounded) multiplication operator on $\mathfrak{h}$ by the k^{th} coordinate x_k:

$$X_k(\psi)(x_1,...,x_d) := x_k\psi(x_1,...,x_d),$$

for ψ in the domain of definition of X_k. The (random) velocity operator in the direction x_k is given by

$$\dot{X}_k := i\left[\Delta_{\omega,\vartheta}^{(\mathbf{A})} + \lambda\omega_1, X_k\right].$$

Note that

$$\Delta_{\omega,\vartheta}^{(\eta\mathbf{A}_\ell)}\mathfrak{e}_x = \sum_{z\in\mathbb{Z}^d,|z|=1}\left\langle \mathfrak{e}_{x+z}, \Delta_{\omega,\vartheta}^{(\eta\mathbf{A}_\ell)}\mathfrak{e}_x\right\rangle_{\mathfrak{h}} \mathfrak{e}_{x+z}$$

and

$$-i\left[\Delta_{\omega,\vartheta}^{(\eta\mathbf{A}_\ell)}, X_k\right]\mathfrak{e}_x = i\left(\left\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}^{(\eta\mathbf{A}_\ell)}\mathfrak{e}_x\right\rangle_{\mathfrak{h}} \mathfrak{e}_{x+e_k} - \left\langle \mathfrak{e}_{x-e_k}, \Delta_{\omega,\vartheta}^{(\eta\mathbf{A}_\ell)}\mathfrak{e}_x\right\rangle_{\mathfrak{h}} \mathfrak{e}_{x-e_k}\right).$$

Moreover, by Equation (4.32),

$$\mathcal{J}_\ell^{(\omega)} = \frac{i}{|\Lambda_\ell|}\sum_{x\in\Lambda_\ell}\left\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}^{(\eta\mathbf{A}_\ell)}\mathfrak{e}_x\right\rangle_{\mathfrak{h}} P_{\{x+e_k\}}s_{e_k}P_{\{x\}} - \frac{i}{|\Lambda_\ell|}\sum_{x\in\Lambda_\ell}\left\langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}^{(\eta\mathbf{A}_\ell)}\mathfrak{e}_{x+e_k}\right\rangle_{\mathfrak{h}} P_{\{x\}}s_{-e_k}P_{\{x+e_k\}}.$$

Therefore, one obtains that

$$\mathcal{J}_\ell^{(\omega)} = -|\Lambda_\ell|^{-1}P_{\Lambda_\ell}\left(i\left[\Delta_{\omega,\vartheta}^{(\eta\mathbf{A}_\ell)} + \lambda\omega_1, X_k\right]\right)P_{\Lambda_\ell} + \mathcal{O}(\ell^{-1}).$$

uniformly with respect to all parameters. By applying the state $\varrho_t^{(\omega,\lambda,\mathbf{A})}$ to $\mathcal{J}_\ell^{(\omega)}$, one recovers the formulation in [13, Equation 2.6] for the thermodynamic limit (large ℓ). Indeed, one gets

$$\varrho_t^{(\omega,\lambda,\mathbf{A})}\left(\mathcal{J}_\ell^{(\omega)}\right) = -|\Lambda_\ell|^{-1}\mathrm{Tr}_{\mathfrak{h}}\left(S_{t,s}^{(\omega,\lambda,\mathbf{A})}P_{\Lambda_\ell}i\left[\Delta_{\omega,\vartheta}^{(\eta\mathbf{A}_\ell)} + \lambda\omega_1, X_k\right]P_{\Lambda_\ell}\right) + \mathcal{O}(\ell^{-1}).$$

Recall that the velocity operator is given by $i[\Delta_{\omega,\vartheta}^{(\eta\mathbf{A}_\ell)} + \lambda\omega_1, X_k]$. Note that electric fields accelerate charged particles and induce so–called diamagnetic currents, which correspond to the ballistic movement of particles. On the other hand, paramagnetic current is intrisinc to the system without perturbation. This is related to heat production. For more details, see [33, Sections 3 and 4].

Currents Density: To shortly present how the linear response current naturally appears, without requiring a thorough reading of Bru-de Siqueira Pedra-Hertling's series of papers, consider now a space homogeneous electric fields in the box Λ_L (4.8) for any $L \in \mathbb{R}^+$. To be more precise, let $\mathcal{A} \in C_0^\infty(\mathbb{R};\mathbb{R}^d)$ and set $\mathcal{E}(t) \doteq -\partial_t\mathcal{A}(t)$ for all $t \in \mathbb{R}$. Therefore, $\mathbf{A}$ is defined to be the vector potential such that the electric field is given by $\mathcal{E}(t) \in C_0^\infty(\mathbb{R};\mathbb{R}^d)$ at time $t \in \mathbb{R}$, for all $x \in [-1,1]^d$, and $(0,0,\ldots,0)$ for $t \in \mathbb{R}$ and $x \notin [-1,1]^d$. It yields a rescaled vector potential $\eta\mathbf{A}_L$, for $L \in \mathbb{R}^+$ and $\eta \in \mathbb{R}_0^+$. See (4.31). Now, let us introduce the current densities induced by the electromagnetic field, that is switched on at time $t_0 = 0 < t$:

Definition 4.3.1 (Current density)
Let $L \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda, \vartheta \in \mathbb{R}_0^+$ $\eta, t \in \mathbb{R}$, $k \in \{1,\ldots,d\}$ and a normalized vector $\overrightarrow{w} := (w_1, ..., w_d) \in \mathbb{R}^d$. The current density response $\mathbb{J}_{\Lambda_L}^{(\omega)}(t,\eta) \in \mathbb{R}^d$ is defined by

$$\mathbb{J}_{\Lambda_L}^{(\omega,\eta\mathbf{A}_\ell)}(t) := \frac{1}{|\Lambda_L|}\sum_{k=1}^{d} w_k \sum_{x\in\Lambda_L}\left(\tau_{t,0}^{(\omega,\lambda,\mathbf{A}_L)}\left(\mathbf{I}_{(x+e_k,x)}^{(\omega,\eta\mathbf{A}_L)}\right) - I_{(x+e_k,x)}^{(\omega)}\right).$$

Following the works that has been done by J.B. Bru , W. de Siqueira Pedra and C. Hertling (see, e.g., [30, Theorem 3.7]), the current density observable satisfies

$$\mathbb{J}_{\Lambda_L}^{(\omega,\eta\mathbf{A}_{\Lambda_L})}(t) = \eta\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}(t) + \mathcal{O}\left(\eta^2\right) \tag{4.33}$$

where

$$\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}(t) := \sum_{k,q=1}^{d} w_k \int_{-\infty}^{0} \{\mathcal{E}(\alpha+t)\}_q \left\{C_{\Lambda_L}^{(\omega)}(t-\alpha)\right\} \mathrm{d}\alpha. \tag{4.34}$$

$C_{\Lambda}^{(\omega)}$ is the conductivity matrix observable within the finite box $\Lambda \subset \mathbb{Z}^d$. Following [30], $C_{\Lambda}^{(\omega)} \in C^1(\mathbb{R};\mathcal{B}(\mathbb{R}^d;\mathcal{U}^d))$, with respect to the canonical orthonormal basis $\{e_q\}_{q=1}^d$ of the Euclidian space $\mathbb{R}^d$, is given by the matrix entries:

$$\left\{C_{\Lambda}^{(\omega)}(t)\right\}_{k,q} := \frac{1}{|\Lambda|} \sum_{x,y,x+e_k,y+e_q\in\Lambda} \int_0^t i[\tau_{-\alpha}^{(\omega)}(I_{(y+e_q,y)}^{(\omega)}), I_{(x+e_k,x)}^{(\omega)}]\mathrm{d}\alpha \tag{4.35}$$

$$+ \frac{2\delta_{k,q}}{|\Lambda|} \sum_{x\in\Lambda} \Re\mathrm{e}\left(\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle a(\mathfrak{e}_{x+e_k})^* a(\mathfrak{e}_x)\right), \tag{4.36}$$

for any $\omega \in \Omega$, $t \in \mathbb{R}$, $\lambda, \vartheta \in \mathbb{R}_0^+$ and $k, q \in \{1, \ldots, d\}$. Recall that $[A, B] := AB - BA \in \mathcal{U}$ denotes the commutator of the elements $A, B \in \mathcal{U}$. By using a generalization of *Lieb-Robinson Bound* for multicommutators [31], Bru and de Siqueira Pedra prove in the general (possibly interacting) case that the residual term $\mathcal{O}(\eta^2)$ in Equation (4.33) is uniformly bounded for $\ell \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda, t, \vartheta \in \mathbb{R}_0^+$. In [29, 31], they give a proof of the existence of the limit of the linear response current density $\varrho^{(\omega)}(\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}(t))$, for $L \to \infty$ and $t \in \mathbb{R}$, to a deterministic value. By using standard tools in probability theory (Large Deviation Principle), see Chapter 5, we sharpen this result by showing an exponential suppression of quantum uncertainty around the macroscopic (classical) current densities.

4.3.3 Discussion on the heat transport for free fermions in a disordered media

Knowing the linear response in terms of currents to electric fields, it is natural to rise the issue of the derivation of the celebrated Heat equation, first introduced by *J. Fourier* in 1807, from the principles of quantum mechanics. The idea is the following: one imposes an electromagnetic field on a small box to heat the system. Then, we analyze the heat production away from this box, i.e., how the energy of a finite region increases with respect to time and the distance from the box when the electromagnetic field is switched off. To this end, one can use all the previous mathematical setting.

The effect of an electromagnetic potential leads to a pertubation of the free dynamics, as explained in previous sections. On can study the energy propagation in a finite ring contained in $\mathbb{Z}^d$, like for instance, at fixed $\ell \in \mathbb{R}^+$, $r \in (1, \infty)$, $\tilde{r} \in \mathbb{R}^+$ and $\zeta \in [0, 1)$,

$$\mathcal{R}_\ell := \left\{x \in \mathbb{Z}^d : r\ell \le |x|^{-1} \le \left(r + \tilde{r}\ell^{-\zeta}\right)\ell\right\}. \tag{4.37}$$

Note that $\mathcal{R}_\ell \cap \Lambda_\ell = \emptyset$. The first step is then to compute the energy density increment

$$\epsilon^{(\omega)}_{\mathcal{R}_\ell}(\eta, t) := \tau^{(\omega,\eta\mathbf{A}_\ell)}_{t,0}\left(\mathfrak{E}^{(\omega)}_{\mathcal{R}_\ell}\right) - \tau^{(\omega)}_{t}\left(\mathfrak{E}^{(\omega)}_{\mathcal{R}_\ell}\right) \tag{4.38}$$

induced at any time $t \in \mathbb{R}$ by electric fields that are switched *on* at time $t = 0$ and switch off at time $T > 0$ (cyclic electromagnetic process, see Definition 2.1.2) and computed from the density energy observable

$$\mathfrak{E}^{(\omega)}_{\mathcal{R}_\ell} := \frac{1}{|\mathcal{R}_\ell|}\sum_{x,y\in\mathcal{R}_\ell}\langle \mathfrak{e}_x, h^{(\omega)}\mathfrak{e}_y\rangle a^*(\mathfrak{e}_x)a(\mathfrak{e}_y)$$

within the ring $\mathcal{R}_\ell$. This has to be done as a function of the parameter $\eta \in \mathbb{R}^+_0$, uniformly with respect to $|\mathcal{R}_\ell|$ and $\omega \in \Omega$. Provided it exists, the limit energy density increment, defined by

$$\epsilon(\eta, t) := \lim_{\ell\to\infty}\varrho^{(\omega)}\left(\epsilon^{(\omega)}_{\mathcal{R}_\ell}(\eta, t)\right),$$

has then to be computed for sufficiently small η. Similar to the derivation of the AC-conductivity measure derived in [29], one can consider the case $t > T$, when the electric fields is switched off.

For any $n \in \mathbb{N}$, we already know that the energy density increment $\epsilon^{(\omega)}_{\mathcal{R}_\ell}(\eta, t)$ can be approximated as a power series in $\eta \in \mathbb{R}^+_0$:

$$\epsilon^{(\omega)}_{\mathcal{R}_\ell}(\eta, t) = \sum_{k=1}^{n}\eta^k\mathbf{E}^{(\omega)}_{k,t,\ell} + \mathcal{O}(\eta^n)$$

uniformly with respect to $\omega \in \Omega$, $\lambda, \ell \in \mathbb{R}^+$, ϑ and t in compact sets, by Taylor's theorem for increments [31, Theorem 4.15], which is in fact a consequence of the Lieb Robinson bound for multi-commutators (see, e.g., [31, Corollary 4.12]). The random element $\mathbf{E}^{(\omega)}_{k,t,\ell}$ does not depend on $\eta \in \mathbb{R}^+_0$. Of course to prove the existence of the limit $\epsilon(\eta)$, one has to use the ergodicity of the distribution $\mathfrak{a}_\Omega$ together with the Akcoglu–Krengel ergodic theorem (see, e.g. [37, Definition VI.1.6]). An explicit expression of the coefficients $\mathbf{E}^{(\omega)}_{1,t,\ell}$ and $\mathbf{E}^{(\omega)}_{2,t,\ell}$ and their time-derivative can be directly deduced from Lemmata 7.8.2 and 7.8.4 together with (7.89) and the trivial asymptotic

$$\mathrm{e}^{\eta x} = 1 + \eta + \frac{\eta^2}{2} + \mathcal{O}\left(\eta^2\right),$$

as $\eta \to 0$. By Lemma 7.8.3, note that $\mathbf{E}^{(\omega)}_{1,t,\ell}$ vanishes, as $\ell \to \infty$. Similar to Ohm's law, which is directly related the η^2-coefficients, we expect that the heat equation is reflected in the coefficient $\mathbf{E}^{(\omega)}_{2,t,\ell}$, but in rescaled space-time parameters, r and time $\mathbf{t} = t\ell^\eta \gg T$ for some appropriate parameter $\xi \in \mathbb{R}^+_0$. Indeed, since the distance between the ring $\mathcal{R}_\ell$ and the box increase Λ_ℓ like $\mathcal{O}(\ell)$, as $\ell \to \infty$, we need an infinite microscopic time t to transport the heat produced by the electromagnetic field from the box to the ring. The time $\mathbf{t} = t\ell^{\eta}$ can be interpreted as a macroscopic time.

Clearly, the main case of interest is the case $\vartheta = 0$, meaning that the second parameter ω_2 in $\Omega := [-1,1]^{\mathbb{Z}^d} \times \mathbb{D}^{\mathfrak{b}}$ is not taken into account. In this case, the one-particle Hamiltonian is given by the random Shrödinger operator

$$h^{(\omega)}|_{\vartheta=0} = \Delta_{\mathrm{d}} + \lambda\omega_1, \quad (\omega_1, \omega_2) \in \Omega,\ \lambda \in \mathbb{R}_0^+,$$

where $\omega_1 : \mathbb{Z}^d \to [-1,1]$ is identified with the corresponding (self-adjoint) multiplication operator and $\Delta_{\mathrm{d}} \in \mathcal{B}(\mathfrak{h})$ is (up to a minus sign) the usual d–dimensional discrete Laplacian:

$$[\Delta_{\mathrm{d}}(\psi)](x) := 2d\psi(x) - \sum_{z\in\mathfrak{L},\ |z|=1} \psi(x+z)\,, \qquad x \in \mathfrak{L},\ \psi \in \mathfrak{h}\,. \tag{4.39}$$

See (4.6) and (4.7) for $\vartheta = 0$. Note that, for an independent identically distributed (i.i.d.) random potential ω_1, $h^{(\omega)}$ is the celebrated Anderson tight–binding model acting on the Hilbert space $\mathfrak{h}$, widely used in mathematics and in physics.

Even for $\vartheta = 0$, the derivation of the heat equation turns out to be quite involved. The difficulty is that this property refers to a regime for which one needs an "Anderson delocalization", i.e., the inverse of the celebrated Anderson localization, to be able to extract some heat equation from the approximated energy density. This is still an open problem.

Chapter 5

Large Deviation Principle for the Conductivity of Free Fermions

5.1 Preliminary presentation of Large Deviation in the Algebraic Formulation of quantum mechanics

In probability theory, the law of large numbers refers to the convergence (at least in probability), as $n \to \infty$, of the average or empirical mean of n independent identically distributed (i.i.d.) random variables towards their expected value (assuming it exists). The large deviation formalism quantitatively describes, for large $n \gg 1$, the probability of finding an empirical mean that differs from the expected value. These are *rare* events and the LD principle (LDP) gives their probability as exponentially small (with respect to some speed) in the limit $n \to \infty$. In the context of the algebraic formulation of quantum mechanics, *observables* (i.e., self-adjoint elements of some C^*-algebra, here $\mathcal{U}$) generalize the notion of random variables of classical probability theory. The link between both notions is given via the Riesz-Markov theorem and functional calculus. Indeed, the commutative C^*-subalgebra of $\mathcal{U}$ generated by any self-adjoint element $A^* = A \in \mathcal{U}$ is isomorphic to the algebra of continuous functions on the compact set $\mathrm{spec}(A) \subset \mathbb{R}$. Therefore, by the Riesz-Markov theorem, for any state ρ, there is a unique probability measure $\mathfrak{m}_{\rho,A}$ on $\mathbb{R}$ such that

$$\mathfrak{m}_{\rho,A}(\mathrm{spec}(A)) = 1 \qquad \text{and} \qquad \rho\left(f(A)\right) = \int_{\mathbb{R}} f(x)\mathfrak{m}_{\rho,A}(\mathrm{d}x) \tag{5.1}$$

for all complex-valued continuous functions $f \in C(\mathbb{R};\mathbb{C})$. $\mathfrak{m}_{\rho,A}$ is called the *distribution* of the *observable* A in the state ρ. As it is mentioned above, the large deviation (LD) formalism describes, for large $n \gg 1$, the probability of finding an empirical mean that differs from the expected value. In Section 5.2, we apply this theory to prove the exponentially fast convergence of microscopic current densities towards their (classical) macroscopic values. For completeness, we present the main result from LD theory used in the current study, namely, the Gärtner-Ellis theorem (Theorem 5.1.1 below). For more details, see [38, 39]. For a historical review of LD in quantum statistical mechanics, see [18, Section 7.1].

Let $\mathcal{X}$ denote a topological vector space. A lower semi-continuous function $\mathrm{I}:\mathcal{X}\to[0,\infty]$ is called a *good rate function* if I is not identically ∞ and has compact level sets, i.e., $\mathrm{I}^{-1}([0,m])=\{x\in\mathcal{X}:\mathrm{I}(x)\leq m\}$ is compact for any $m\geq 0$. A sequence $(X_L)_{L\in\mathbb{N}}$ of $\mathcal{X}$-valued random variables satisfies the *LD upper bound* with *speed* $(\mathfrak{n}_L)_{L\in\mathbb{N}}\subset\mathbb{R}^+$ (a positive, increasing and divergent sequence) and rate function I if, for any closed subset F of $\mathcal{X}$,

$$\limsup_{L\to\infty}\frac{1}{\mathfrak{n}_L}\ln\mathbb{P}(X_l\in F)\leq-\inf_{x\in F}\mathrm{I}(x), \tag{5.2}$$

and it satisfies the *LD lower bound* if, for any open subset G of $\mathcal{X}$,

$$\liminf_{L\to\infty}\frac{1}{\mathfrak{n}_L}\ln\mathbb{P}(X_l\in G)\geq-\inf_{x\in G}\mathrm{I}\,(x)\,. \tag{5.3}$$

If both, upper and lower bound, are satisfied, one says that $(X_L)_{L\in\mathbb{N}}$ satisfies an *LD principle* (LDP). The principle is called *weak* if the upper bound in (5.2) holds only for *compact* sets F.

A weak LDP can be strengthened to a full one by showing that the sequence $(X_L)_{L\in\mathbb{N}}$ of distributions is *exponentially tight*, i.e., if for any $\alpha\in\mathbb{R}$, there is a compact subset $\mathcal{G}_\alpha$ of $\mathcal{X}$ such that

$$\limsup_{L\to\infty}\frac{1}{\mathfrak{n}_L}\ln\mathbb{P}(X_L\in\mathcal{X}\backslash\mathcal{G}_\alpha)<-\alpha. \tag{5.4}$$

If $\mathcal{X}$ is a locally compact topological space, i.e., every point possesses a compact neighborhood, then the existence of an LDP with a good rate function I for the sequence $(X_L)_{L\in\mathbb{N}}$ implies its exponential tightness [39, Exercise 1.2.19].

A sufficient condition to ensure that a sequence $(X_L)_{L\in\mathbb{N}}$ of $\mathcal{X}$-valued random variables satisfies an LDP is given by the Gärtner-Ellis theorem. It says [39, Corollary 4.5.27] that an exponentially tight sequence $(X_L)_{L\in\mathbb{N}}$ of $\mathcal{X}$-valued random variables on a Banach space $\mathcal{X}$ satisfies an LDP with the good rate function

$$\mathrm{I}\,(x)=\sup_{s\in\mathcal{X}^*}\{s\,(x)-J(s)\}\ ,\qquad x\in\mathcal{X}, \tag{5.5}$$

whenever the so-called limiting logarithmic moment generating function

$$J(s)\doteq\lim_{L\to\infty}\frac{1}{\mathfrak{n}_L}\ln\mathbb{E}\left[\mathrm{e}^{\mathfrak{n}_L s(X_L)}\right]\ ,\qquad s\in\mathcal{X}^*, \tag{5.6}$$

exists as a Gateaux differentiable and weak* lower semi-continuous (finite-valued) function on the dual space $\mathcal{X}^*$. See also [38, Theorem 2.2.4].

The random variables we study here result from bounded sequences $(A_L)_{L\in\mathbb{N}}\subset\mathcal{U}$ of self-adjoint elements of the CAR C^*-algebra $\mathcal{U}$ with some fixed state $\rho\in\mathcal{U}^*$. Via the Riesz-Markov theorem and functional calculus, see Equation (5.1), such a sequence and state naturally define an exponentially tight sequence of random variables on the real line $\mathcal{X}=\mathbb{R}$, . The following simple version of the celebrated Gärtner-Ellis theorem of LD theory is sufficient for our purposes:

Theorem 5.1.1 (Gärtner-Ellis)
Take any exponentially tight sequence $(X_L)_{L\in\mathbb{N}}$ of real-valued random variables (i.e., $\mathcal{X} = \mathcal{X}^* = \mathbb{R}$) and assume that the limiting logarithmic moment generating function J defined by (5.6) exists for all $s \in \mathbb{R}$. Then:
(LD1) $(X_L)_{L\in\mathbb{N}}$ *satisfies the LD upper bound (5.2) with rate function* I *given by (5.5).*
(LD2) *If, additionally,* J *is differentiable for all $s \in \mathbb{R}$ then $(X_L)_{L\in\mathbb{N}}$ satisfies the LD lower bound (5.3) with good rate function* I *given again by (5.5).*

Proof: (LD1) and (LD2) are special cases of [43, Theorem V.6.(a) and (c)] , respectively. ■

5.2 Exponential suppression of quantum effects around the classical macroscopic current values

Recall the setting of Section 4.3.2: Let $\mathcal{A} \in C_0^\infty(\mathbb{R};\mathbb{R}^d)$ and set $\mathcal{E}(t) \doteq -\partial_t\mathcal{A}(t)$ for all $t \in \mathbb{R}$. Therefore, $\mathbf{A}$ is defined to be the vector potential such that the electric field is given by $\mathcal{E}(t) \in C_0^\infty(\mathbb{R};\mathbb{R}^d)$ at time $t \in \mathbb{R}$, for all $x \in [-1,1]^d$, and $(0,0,\ldots,0)$ for $t \in \mathbb{R}$ and $x \notin [-1,1]^d$. It yields a rescaled vector potential $\eta\mathbf{A}_L$, for $L \in \mathbb{R}^+$ and $\eta \in \mathbb{R}_0^+$. See (4.31). Then, the current linear response current density induced by the electromagnetic field, that is switched on at time $t_0 = 0 < t$, is equal to

$$\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}(t) := \sum_{k,q=1}^{d} w_k \int_{-\infty}^{0} \{\mathcal{E}(\alpha+t)\}_q \left\{C_{\Lambda_L}^{(\omega)}(t-\alpha)\right\} \mathrm{d}\alpha,$$

for any $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$, by (4.33). See also (4.35). Note that in [30], the result is mentioned with $\mathcal{E} \in C_0^\infty(\mathbb{R};\mathbb{R}^d)$, however this condition $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ appears to be enough in the formulation of our results.

For any fixed time $t \in \mathbb{R}$, we study large deviations (LD) for the family $\{\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}(t)\}_{\ell\in\mathbb{R}^+}$ produced by any fixed, time-dependent electric field $\mathcal{E}$. To this end, it suffice to consider the case $t = 0$ because it suffices to replace $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ in the definition of $\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}(0)$ with

$$\mathcal{E}_t(\alpha) \doteq \mathcal{E}(\alpha+t), \qquad \alpha \in \mathbb{R}.$$

in order to obtain the current density $\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}(t)$ at any time $t \in \mathbb{R}$. So, from now, we define

$$\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})} := \mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}(0)$$

for any $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$. The large deviations (LD) for the family $\{\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}\}_{L\in\mathbb{R}^+}$ is a consequence of the Gärtner-Ellis theorem, see Theorem 5.1.1, combined with the following result:

Theorem 5.2.1 (Generating functions for currents)
There is a measurable subset $\tilde{\Omega} \subset \Omega$ of full measure such that, for all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \tilde{\Omega}$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ and $\vec{w} \in \mathbb{R}^d$ with $\left\|\vec{w}\right\|_{\mathbb{R}^d} = 1$, the limit

$$\lim_{L\to\infty} \frac{1}{|\Lambda_L|} \ln \varrho^{(\omega)} \left(\mathrm{e}^{|\Lambda_L| \mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}} \right)$$

exist and equals

$$\mathrm{J}^{(\mathcal{E})} := \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \mathbb{E}\left[\ln \varrho^{(\cdot)} \left(\mathrm{e}^{|\Lambda_L| \mathbb{I}_{\Lambda_L}^{(\cdot,\mathcal{E})}} \right) \right].$$

Moreover, for any $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$, the map $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ from $\mathbb{R}$ to itself is continuously differentiable and convex.

Proof: The assertions directly follow from Corollaries 7.5.4 and 7.5.5. Note that the map $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ is a limit of convex functions, and hence, it is also convex. This result is obtained by doing a decomposition of the current density within a box Λ_L into a sum of current density of small boxes contained in Λ_L. Afterwards, one relies on the property of ergodicity (Ackoglu-Krengel ergodic theorem) in order to obtain the fact the sum of the current densities within small boxes is nothing but its expectation value. One of the key points of the box decomposition is that we have to control the norm of

$$\mathrm{e}^{uH_\alpha} \{\partial_\alpha H_\alpha\} \mathrm{e}^{-uH_\alpha}, \quad H_\alpha \in \mathcal{U}$$

Indeed, while doing the decomposition of a box Λ_L, one has a error given by the following *Bogoliubov* type inequality:

$$\left| \ln \mathrm{tr}\left(C\mathrm{e}^{H_1} \right) - \ln \mathrm{tr}\left(C\mathrm{e}^{H_0} \right) \right| \leq \sup_{\alpha\in[0,1]} \sup_{u\in[-1/2,1/2]} \left\| \mathrm{e}^{u(\alpha H_1 + (1-\alpha)H_0)} (H_1 - H_0)\, \mathrm{e}^{-u(\alpha H_1+(1-\alpha)H_0)} \right\|_{\mathcal{U}}.$$

In general, there is no result on which one can rely to control the norm of above quantity. Nevertheless, in the context of our problem, we deal quasi-free state on one hand. And on the other hand, we will see in the sequel that H_α is a bilinear element. The combination of both facts will leads us to a very good control of above quantity.

Finally, we use the Arzelà-Ascoli theorem to ensure the fact that the map $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ from $\mathbb{R}$ to itself is continuously differentiable. ■

A large deviation principle for currents is then a direct consequence of Theorems 5.1.1 and Theorem 5.2.1:

Corollary 5.2.1 (Large deviation principle for currents)
Let $\tilde{\Omega} \subset \Omega$ be the measurable subset of full measure of Theorem 5.2.1. Then, for all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \tilde{\Omega}$, $l \in \mathbb{N}$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ and $\vec{w} \in \mathbb{R}^d$ with $\left\|\vec{w}\right\|_{\mathbb{R}^d} = 1$, the sequence $\{\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}\}_{L\in\mathbb{R}^+}$ of microscopic current densities satisfies a Large Deviation Principle, in the KMS state $\varrho^{(\omega)}$, with speed $|\Lambda_L|$ and good rate function $\mathrm{I}^{(\mathcal{E})}$ defined on $\mathbb{R}$ by

$$\mathrm{I}^{(\mathcal{E})}(x) := \sup_{s\in\mathbb{R}} \left\{ sx - \mathrm{J}^{(s\mathcal{E})} \right\} \geq 0.$$

Remark 5.2.2
By direct estimates, one verifies that, for any fixed state ρ, $\{\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}\}_{L\in\mathbb{R}^+}$ *yields an exponentially tight family of probability measures, defined by (5.1) for* $A = \mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}$. *Therefore, by [39, Lemma 4.1.23],* $\{\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}\}_{L\in\mathbb{R}^+}$ *satisfies, along some subsequence, an LDP,* in any state ρ, *with speed* $|\Lambda_L|$ *and a good rate function. However, it is not clear whether this rate function depends on the choice of subsequences and* $\omega \in \Omega$. *Moreover, no information on minimizers of the rate function, like in Theorem 5.2.2, can be deduced from [39, Lemma 4.1.23].*

Therefore, by [34, 29] and Corollary 5.2.1, the distributions of the microscopic current density observables, in the state $\varrho^{(\omega)}$, weak* converges, for $\omega \in \Omega$ almost surely, to the delta distribution at the (classical value of the) macroscopic current density. Using Theorem 5.2.1, we sharpen this result by proving that the microscopic current density converges *exponentially fast* to the macroscopic one, with respect to the volume $|\Lambda_L|$ of the region of the lattice where an external electric field is applied. To this end, we remark from (7.58) that, for any $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\vec{w} \in \mathbb{R}^d$ with $\left\|\vec{w}\right\|_{\mathbb{R}^d} = 1$, the macroscopic current density is equal to

$$x^{(\mathcal{E})} := \partial_s \mathrm{J}^{(s\mathcal{E})}|_{s=0}, \quad \mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d). \tag{5.7}$$

Define

$$x_- := \inf\left\{x \leq x^{(\mathcal{E})} : \mathrm{I}^{(\mathcal{E})}(x) < \infty\right\},\ x_+ := \sup\left\{x \geq x^{(\mathcal{E})} : \mathrm{I}^{(\mathcal{E})}(x) < \infty\right\}.$$

Obviously, $\mathrm{I}^{(\mathcal{E})}(x) = \infty$ for $x \in \mathbb{R}\backslash[x_-, x_+]$. We start by giving important properties of the rate function $\mathrm{I}^{(\mathcal{E})}$:

Theorem 5.2.2 (Properties of the rate function)
Fix $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\vec{w} \in \mathbb{R}^d$ *with* $\left\|\vec{w}\right\|_{\mathbb{R}^d} = 1$ *and* $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$. *The rate function* $\mathrm{I}^{(\mathcal{E})}$ *is a lower-semicontinuous convex function satisfying:*

i) $\mathrm{I}^{(\mathcal{E})}(x^{(\mathcal{E})}) = 0$;

ii) $\mathrm{I}^{(\mathcal{E})}(x) > 0$ *if* $x \neq x^{(\mathcal{E})}$;

iii) $\mathrm{I}^{(\mathcal{E})}(x) < \infty$ *for* $x \in (x_-, x_+)$ *with* $\mathrm{I}^{(\mathcal{E})}(x) \leq \mathrm{I}^{(\mathcal{E})}(x_-)$ *for* $x \in (x_-, x^{(\mathcal{E})}]$ *and* $\mathrm{I}^{(\mathcal{E})}(x) \leq \mathrm{I}^{(\mathcal{E})}(x_+)$ *for* $x \in [x^{(\mathcal{E})}, x_+)$;

iv) $\mathrm{I}^{(\mathcal{E})}$ *restricted to the interior of its domain, i.e., the (possibly empty) open interval* (x_-, x_+), *is continuous.*

Proof: Fix all parameters of the theorem. Note that $\mathrm{I}^{(\mathcal{E})}$ is clearly a lower-semicontinuous convex function, by construction. As the map $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ is differentiable and convex (Theorem 5.2.1), the map $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ is the Legendre-Fenchel transform of $\mathrm{I}^{(\mathcal{E})}$, i.e.,

$$\mathrm{J}^{(s\mathcal{E})} = \sup_{x\in\mathbb{R}}\left\{sx - \mathrm{I}^{(\mathcal{E})}(x)\right\}, \qquad s \in \mathbb{R},$$

and s_0 is a solution of the variational problem

$$\mathrm{I}^{(\mathcal{E})}(x) := \sup_{s\in\mathbb{R}} \left\{ sx - \mathrm{J}^{(s\mathcal{E})} \right\}$$

if and only if s_0 solves $x = \partial_s \mathrm{J}^{(s\mathcal{E})}|_{s=s_0}$. By (5.7), it follows that

$$0 = \mathrm{J}^{(0)} = \inf_{x\in\mathbb{R}} \mathrm{I}^{(\mathcal{E})}(x) = \mathrm{I}^{(\mathcal{E})}(x^{(\mathcal{E})}).$$

This proves Assertion *(i)*.

To prove *(ii)*, it suffices to show that $x^{(\mathcal{E})}$ is the only minimizer of $\mathrm{I}^{(\mathcal{E})}$. Note that x_0 is a minimizer of $\mathrm{I}^{(\mathcal{E})}$ if and only if 0 is a subdifferential of $\mathrm{I}^{(\mathcal{E})}$ at x_0 (Fermat's principle). By [49, Corollary 5.3.3] and the differentiability of the Legendre transform of $\mathrm{I}^{(\mathcal{E})}$, which is the map $s \mapsto \mathrm{J}^{(s\mathcal{E})}$, it follows that the minimizer of $\mathrm{I}^{(\mathcal{E})}$ is unique and Assertion *(ii)* follows.

Assertion *(iii)* is a direct consequence of the fact that $\mathrm{I}^{(\mathcal{E})}$ is a convex function with $x^{(\mathcal{E})}$ as unique minimizer.

Assertion *(iv)* is deduced from *(i)*, *(ii)* and [49, Corollary 2.1.3]. ■

Corollary 5.2.3 (Exponentially fast suppression of quantum uncertainty of currents)
Let $\tilde{\Omega} \subset \Omega$ be the measurable subset of full measure of Theorem 5.2.1. Then, for all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \tilde{\Omega}$, $l \in \mathbb{N}$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$, $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$, and any open subset $\mathcal{O} \subset \mathbb{R}$ with $x^{(\mathcal{E})} \notin \bar{\mathcal{O}}$,

$$\limsup_{L\to\infty} \frac{1}{|\Lambda_L|} \ln \mathfrak{m}_{\varrho^{(\omega)},\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}} (\mathcal{O}) < 0.$$

The above limit does not depend on the particular realization of $\omega \in \tilde{\Omega}$. If, additionally, $\mathcal{O} \cap (x_-, x_+) \neq \emptyset$, then

$$\lim_{L\to\infty} \frac{1}{|\Lambda_L|} \ln \mathfrak{m}_{\varrho^{(\omega)},\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}} (\mathcal{O}) = -\inf_{x\in\mathcal{O}} \mathrm{I}^{(\mathcal{E})}(x) < 0.$$

See (5.1) for the definition of the distribution of $\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}$, in the KMS state $\varrho^{(\omega)}$.

Proof: It is a direct consequence of Corollary 5.2.1 and Theorem 5.2.2. ■

Corollary 5.2.3 shows that the microscopic current density converges *exponentially fast* to the macroscopic one, with respect to the volume $|\Lambda_L|$ (in lattice units (l.u.)) of the region of the lattice where the electric field is applied. As discussed in the introduction, this is in accordance with the low temperature (4.2K) experiment [58] on the resistance of nanowires with lengths down to approximately 20 l.u. ($L \simeq 10$).

To conclude, note that, in the experimental setting of [60, 58], contacts are used to impose an electric potential difference to the nanowires. These contacts yield supplementary resistances to the system that are well-described by Landauer's formalism [46] when a *ballistic* charge transport takes place in the nanowires. In our model, the purely ballistic charge transport is reached when $\vartheta = 0$ and $\lambda \to 0^+$, as proven in [32, Theorem 4.6]. When the nanowire resistance becomes relatively small as compared to the contact resistances, then the charge transport in the nanowire is well-described by a ballistic approximation and Landauer's formalism applies, as also experimentally verified in [60]. This is the reason why [58] reaches much smaller length scales than [60]: the material used in [58] has a much larger linear resistivity (about $1000\Omega/nm$, see [58, Fig. 1 E]) than the one of [60] ($23\Omega/nm$, see [60, discussions after Eq. (2)]).

5.3 Continuity of the generating functions for currents

By Theorem 5.2.1, for all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$,

$$\mathrm{J}_{\vartheta,\lambda}^{(\mathcal{E})} \equiv \mathrm{J}^{(\mathcal{E})} := \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \mathbb{E}\left[\ln \varrho^{(\cdot)} \left(\mathrm{e}^{|\Lambda_L| \mathbb{I}_{\Lambda_L}^{(\cdot,\mathcal{E})}} \right) \right] . \tag{5.8}$$

A question that naturally arises is the continuity of this generating function for currents with respect to the strength $\vartheta, \lambda \in \mathbb{R}_0^+$ of the disorder in the media. This is a priori a *non-trivial* issue: Recall that $\varrho_{\Lambda_{L_\varrho}}^{(\omega)}$ is the quasi-free state with symbol

$$(1 + \mathrm{e}^{\beta h_{\Lambda_{L_\varrho}}^{(\omega)}})^{-1}$$

where $h_{\Lambda_{L_\varrho}}^{(\omega)} := P_{\Lambda_{L_\varrho}} h^{(\omega)} P_{\Lambda_{L_\varrho}}$ (see (4.10)) and $P_{\Lambda_{L_\varrho}}$ is the orthogonal projection defined on $\mathfrak{h}$ by (4.9). By Propositions 3.2.13 and 4.1.1, $\varrho_{\Lambda_{L_\varrho}}^{(\omega)}$ converges, as $L_\varrho \to \infty$, in the weak* topology to $\varrho^{(\omega)}$, while, by Lemma 3.2.12,

$$\varrho_{\Lambda_{L_\varrho}}^{(\omega)}(B) = \frac{\mathrm{tr}\left(B \mathrm{e}^{-\beta H_{L_\varrho}^{(\vartheta,\lambda)}} \right)}{\mathrm{tr}\left(\mathrm{e}^{-\beta H_{L_\varrho}^{(\vartheta,\lambda)}} \right)}, \qquad B \in \mathcal{U},$$

where, by (4.7),

$$H_{L_\varrho}^{(\vartheta,\lambda)} := \left\langle \mathrm{A}, h_{\Lambda_{L_\varrho}}^{(\omega)} \mathrm{A} \right\rangle = \sum_{x,y\in\Lambda_{L_\varrho}} \left\langle \mathfrak{e}_x, [\Delta_{\omega,\vartheta} + \lambda\omega_1]\, \mathfrak{e}_y \right\rangle_{\mathfrak{h}} a^*(\mathfrak{e}_x) a(\mathfrak{e}_y). \tag{5.9}$$

See Definition 3.2.2. In particular, for all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$, it is easy to see that

$$\mathrm{J}_{\vartheta,\lambda}^{(\mathcal{E})} = \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \mathbb{E}\left[\lim_{L_\varrho\to\infty} \left(\ln \mathrm{tr}\left(\mathrm{e}^{|\Lambda_L| \mathbb{I}_{\Lambda_L}^{(\cdot,\mathcal{E})}} \mathrm{e}^{-\beta H_{L_\varrho}^{(\vartheta,\lambda,\omega)}} \right) - \ln \mathrm{tr}\left(\mathrm{e}^{-\beta H_{L_\varrho}^{(\vartheta,\lambda,\omega)}} \right) \right) \right]. \tag{5.10}$$

In order to study the continuity of the map $(\vartheta,\lambda)\mapsto \mathrm{J}^{(\omega,\mathcal{E})}$ from $\mathbb{R}_0^+\times\mathbb{R}_0^+$ to $\mathbb{R}$, one could thus try to use Lemma 7.2.3 (ii), which implies, for any $C\in\mathcal{U}$ and $\vartheta_2,\vartheta_1,\lambda_2,\lambda_1\in\mathbb{R}_0^+$, that

$$\left|\ln\mathrm{tr}\left(C\mathrm{e}^{-\beta H_{L_\varrho}^{(\vartheta_1,\lambda_1)}}\right)-\ln\mathrm{tr}\left(C\mathrm{e}^{-\beta H_{L_\varrho}^{(\vartheta_2,\lambda_2)}}\right)\right| \tag{5.11}$$
$$\leq \sup_{\alpha\in[0,1]}\sup_{u\in[-1/2,1/2]}\left\|\mathrm{e}^{\beta u\left(\alpha H_{L_\varrho}^{(\vartheta_1,\lambda_1)}+(1-\alpha)H_{L_\varrho}^{(\vartheta_2,\lambda_2)}\right)}\beta\left(H_{L_\varrho}^{(\vartheta_1,\lambda_1)}-H_{L_\varrho}^{(\vartheta_2,\lambda_2)}\right)\mathrm{e}^{-u\beta\left(\alpha H_{L_\varrho}^{(\vartheta_1,\lambda_1)}+(1-\alpha)H_{L_\varrho}^{(\vartheta_2,\lambda_2)}\right)}\right\|_{\mathcal{U}}.$$

Since all Hamiltonians in this last expression are self-adjoint bilinear elements, we deduce from (5.11) together with Corollary 3.2.5 and explicit computations using (5.9) (see (5.15) below) that

$$\left|\ln\mathrm{tr}\left(C\mathrm{e}^{-\beta H_{L_\varrho}^{(\vartheta_1,\lambda_1)}}\right)-\ln\mathrm{tr}\left(C\mathrm{e}^{-\beta H_{L_\varrho}^{(\vartheta_2,\lambda_2)}}\right)\right|\leq\mathcal{O}\left(\left|\Lambda_{L_\varrho}\right|\right),$$

which diverges when $L_\varrho\to\infty$. So, these lines of arguments cannot be directly applied to (5.10) in order to prove the continuity of the map $(\vartheta,\lambda)\mapsto\mathrm{J}_{\vartheta,\lambda}^{(\mathcal{E})}$ from $\mathbb{R}_0^+\times\mathbb{R}_0^+$ to $\mathbb{R}$. In fact, in order to obtain that result, one needs to use a *non-trivial* statement deduced from Corollary 7.5.4, that is in this case,

$$\mathrm{J}_{\vartheta,\lambda}^{(\mathcal{E})}=\lim_{L\to\infty}\frac{1}{|\Lambda_L|}\mathbb{E}\left[\left(\ln\mathrm{tr}\left(\mathrm{e}^{|\Lambda_L|\mathbb{I}_{\Lambda_L}^{(\cdot,\mathcal{E})}}\mathrm{e}^{-\beta H_L^{(\vartheta,\lambda,\omega)}}\right)-\ln\mathrm{tr}\left(\mathrm{e}^{-\beta H_L^{(\vartheta,\lambda,\omega)}}\right)\right)\right]. \tag{5.12}$$

Having this in mind, one can then get the following proposition:

Proposition 5.3.1 (Continuity of the generating function with respect to λ and ϑ) *Fix $\beta\in\mathbb{R}^+$, $\vec{w}\in\mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d}=1$ and $\mathcal{E}\in C_0^0(\mathbb{R};\mathbb{R}^d)$. Then, for any $\vartheta_1,\vartheta_2,\lambda_1,\lambda_2\in\mathbb{R}_0^+$,*

$$\left|\mathrm{J}_{\vartheta_1,\lambda_1}^{(\mathcal{E})}-\mathrm{J}_{\vartheta_2,\lambda_2}^{(\mathcal{E})}\right|\leq 2\left(2d\left|\vartheta_1-\vartheta_2\right|+\left|\lambda_1-\lambda_2\right|\right)\beta\mathrm{e}^{\beta(2d(2+\vartheta_2+\vartheta_1)+\lambda_1+\lambda_2)}.$$

In particular, the map $(\vartheta,\lambda)\mapsto\mathrm{J}_{\vartheta,\lambda}^{(\mathcal{E})}$ from $\mathbb{R}_0^+\times\mathbb{R}_0^+$ to $\mathbb{R}$ is jointly continuous.

Proof: By a direct computation, one obtains from (4.6) and (5.9) that, for $\vartheta_2,\vartheta_1,\lambda_2,\lambda_1\in\mathbb{R}_0^+$ and $L=L_\varrho\in\mathbb{N}$,

$$H_{\vartheta_1,\lambda_1}^{(\omega)}-H_{\vartheta_2,\lambda_2}^{(\omega)}=(\vartheta_2-\vartheta_1)\overline{\omega_2(\{x,x-e_j\})}\sum_{x\in\Lambda_L}\sum_{j=1}^{d}a_x^*a_{x+e_j} \tag{5.13}$$
$$+(\vartheta_1-\vartheta_2)\omega_2(\{x,x+e_j\})\sum_{x\in\Lambda_L}\sum_{j=1}^{d}a_x^*a_{x-e_j} \tag{5.14}$$
$$+(\lambda_1-\lambda_2)\sum_{x\in\Lambda_L}\omega_1(x)a_x^*a_x, \tag{5.15}$$

$\{e_k\}_{k=1}^d$ being the canonical orthonormal basis of the Euclidian space $\mathbb{R}^d$. Observe also that, for any $\alpha\in[0,1]$,

$$\alpha H_{\vartheta_1,\lambda_1}^{(\omega)}+(1-\alpha)H_{\vartheta_2,\lambda_2}^{(\omega)}=\langle\mathrm{A},\xi_\alpha\mathrm{A}\rangle$$

is the second quantization of the self-adjoint operator

$$\xi_\alpha := P_{\Lambda_L} \left(\alpha \left(\Delta_{\omega,\vartheta_1} + \lambda_1\omega_1\right) + (1-\alpha)\left(\Delta_{\omega,\vartheta_2} + \lambda_2\omega_1\right)\right) P_{\Lambda_L}$$

whose operator norm is bounded by

$$\sup_{\alpha\in[0,1]} \|\xi_\alpha\|_{\mathcal{B}(\mathfrak{h})} \leq 2d(2+\vartheta_2+\vartheta_1) + \lambda_1 + \lambda_2 \ .$$

Therefore, we deduce from (5.11) together with Corollary 3.2.5 and (5.15) that, for any $C \in \mathcal{U}$ and $\vartheta_2, \vartheta_1, \lambda_2, \lambda_1 \in \mathbb{R}_0^+$,

$$\left|\ln \mathrm{tr}\left(C\mathrm{e}^{-\beta H_L^{(\vartheta_1,\lambda_1)}}\right) - \ln \mathrm{tr}\left(C\mathrm{e}^{-\beta H_L^{(\vartheta_2,\lambda_2)}}\right)\right| \leq \left(2d\,|\vartheta_1-\vartheta_2| + |\lambda_1-\lambda_2|\right)|\Lambda_L|\,\beta\mathrm{e}^{\beta(2d(2+\vartheta_2+\vartheta_1)+\lambda_1+\lambda_2)}.$$

Combined with (5.12), this yields the assertion. ■

In particular, one could approximate the generating function $\mathrm{J}_{\vartheta,\lambda}^{(\mathcal{E})}$ for small $\vartheta, \lambda \ll 1$ by its value at $\vartheta, \lambda = 0$. Note that Proposition 5.3.1 does not imply the continuity of the rate function of Corollary 5.2.1 with respect to $\vartheta, \lambda \in \mathbb{R}_0^+$. This is still not done here because of the lack of time. Instead, we give in the next section an important link between the rate function and the so-called quantum fluctuations.

5.4 Rate function and quantum fluctuations

By Corollary 5.2.1, the (good) rate function $\mathrm{I}^{(\mathcal{E})}$ associated with the LDP of the sequence $\{\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}\}_{L\in\mathbb{R}^+}$ of microscopic current densities, in the KMS state $\varrho^{(\omega)}$ and with speed $|\Lambda_L|$ (Corollary 5.2.1), is defined on $\mathbb{R}$ by

$$\mathrm{I}^{(\mathcal{E})}(x) := \sup_{s\in\mathbb{R}} \left\{sx - \mathrm{J}^{(s\mathcal{E})}\right\} \geq 0. \tag{5.16}$$

In other words, $\mathrm{I}^{(\mathcal{E})}$ is the Legendre-Fenchel transform of the generating function $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ for currents of Theorem 5.2.1. Recall meanwhile from (7.58) that, for any $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\vec{w} \in \mathbb{R}^d$ with $\left\|\vec{w}\right\|_{\mathbb{R}^d} = 1$, the macroscopic current density is equal to

$$x^{(\mathcal{E})} := \partial_s \mathrm{J}^{(s\mathcal{E})}|_{s=0}, \qquad \mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d). \tag{5.17}$$

See (5.7). It equals

$$x^{(\mathcal{E})} = \lim_{L\to\infty} \varrho^{(\omega)}\left(\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}\right)$$

with probability one, i.e., for ω in some measurable subset of full measure. By Theorem 5.2.2, $\mathrm{I}^{(\mathcal{E})}(x^{(\mathcal{E})}) = 0$ and $\mathrm{I}^{(\mathcal{E})}(x) > 0$ if $x \neq x^{(\mathcal{E})}$.

We are interested in knowing the asymptotic behavior of $\mathrm{I}^{(\mathcal{E})}$ around the macroscopic current density $x^{(\mathcal{E})}$. This is directly given via quantum fluctuations of current observables, defined as follows: For any $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$ and $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$, the quantum fluctuation of current observables in a cubic box Λ_L, $L \in \mathbb{R}_0^+$, is defined to be

$$\mathbf{F}_{\Lambda_L}^{(\omega,\mathcal{E})} := |\Lambda_L| \left(\varrho^{(\omega)} \left(\left(\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})} \right)^2 \right) - \varrho^{(\omega)} \left(\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})} \right)^2 \right) ,$$

where we recall that $\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}(t)$ is the current density linear response defined by (4.34). In particular, $|\Lambda_L| \, \mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}(t)$ is linear response in terms of current to the electric field and observe that

$$\mathbf{F}_{\Lambda_L}^{(\omega,\mathcal{E})} = \frac{1}{|\Lambda_L|} \left(\varrho^{(\omega)} \left(\left(|\Lambda_L| \, \mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})} \right)^2 \right) - \varrho^{(\omega)} \left(|\Lambda_L| \, \mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})} \right)^2 \right),$$

which is naturally seen as a a quantum fluctuation of current observables.

We are now in a position to relate the rate function to quantum fluctuations of current observables. Note that this results has not been published yet, since they has been proven after having finished [88].

Theorem 5.4.1 (Quantum fluctuations and rate function)
There is a measurable subset $\tilde{\Omega} \subset \Omega$ of full measure such that, for all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \tilde{\Omega}$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$, the following properties holds true:

(i) The map $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ of Theorem 5.2.1 belongs to $C^2(\mathbb{R},\mathbb{R})$ and satisfies

$$\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} = \lim_{L\to\infty} \mathbb{E}\left[\mathbf{F}_{\Lambda_L}^{(\omega,\mathcal{E})}\right] = \lim_{L\to\infty} \mathbf{F}_{\Lambda_L}^{(\omega,\mathcal{E})}. \tag{5.18}$$

(ii) The rate function $\mathrm{I}^{(\mathcal{E})}$ of Corollary 5.2.1 satisfies the asymptotics

$$\mathrm{I}^{(\mathcal{E})}(x) = \frac{1}{2\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0}} \left(x - x^{(\mathcal{E})}\right)^2 + o\left(\left(x - x^{(\mathcal{E})}\right)^3\right), \tag{5.19}$$

provided that $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} \neq 0$.

Proof: Fix all parameters of the proposition.
(i) By Corollary 7.5.5, the map $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ is a $C^2(\mathbb{R},\mathbb{R})$ function, while (5.18) corresponds to Equation (7.60), which is proven below, in the technical proof section (Chapter 7).
(ii) Since the map $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ from $\mathbb{R}$ to itself is convex and belongs (at least) to $C^1(\mathbb{R},\mathbb{R})$ (see, e.g., Assertion (i) or [88, Theorem 3.1]), all finite solutions $s(x) \in \mathbb{R}$ of the variational problem (5.16) for $x \in \mathbb{R}$, i.e.,

$$\mathrm{I}^{(\mathcal{E})}(x) = s(x)x - \mathrm{J}^{(s(x)\mathcal{E})}, \tag{5.20}$$

satisfies

$$x = f(s(x)), \tag{5.21}$$

with f being the real-valued function defined by

$$f(s) \doteq \partial_s \mathrm{J}^{(s\mathcal{E})}|_s, \qquad s \in \mathbb{R}. \tag{5.22}$$

Assume now that $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} \neq 0$, which is equivalent in this case to

$$\partial_s f(0) = \partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} > 0, \tag{5.23}$$

by positivity of generating functions (see (i)). Since, by Corollary 7.5.5, the mapping $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ from $\mathbb{R}$ to itself belongs to $C^2(\mathbb{R}, \mathbb{R})$, by (5.20)-(5.23) and (5.7), there is an interval

$$\mathcal{I} \subseteq \{f(s) : s \in \mathbb{R} \text{ such that } \partial_s f(s) > 0\} \subseteq \mathbb{R}$$

containing $x^{(\mathcal{E})} = f(0)$ and a well-defined function $x \mapsto s(x)$ from $\mathcal{I}$ to $\mathbb{R}$ such that Equations (5.20)-(5.22) hold true. In particular,

$$\partial_s f(s(x)) = \partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=s(x)} > 0, \qquad x \in \mathcal{I}. \tag{5.24}$$

Observe in this case that the inverse of f is nothing else than

$$s(x) = f^{-1}(x), \qquad x \in \mathcal{I},$$

and, by (5.24), the mapping $x \mapsto s(x)$ from $\mathcal{I}$ to $\mathbb{R}$ is differentiable with derivative given by

$$\partial_x s(x) = \frac{1}{\partial_s f\,(s(x))}, \qquad x \in \mathcal{I}. \tag{5.25}$$

We thus infer from (5.20)-(5.22) and (5.25), together with (i), that

$$\partial_x \mathrm{I}^{(\mathcal{E})}(x) = s(x), \qquad x \in \mathcal{I}.$$

Consequently, $\partial_x \mathrm{I}^{(\mathcal{E})}$ is differentiable on $\mathcal{I}$ with derivative given by

$$\partial_x^2 \mathrm{I}^{(\mathcal{E})}(x) = \partial_x s(x), \qquad x \in \mathcal{I}.$$

As a consequence, $\mathrm{I}^{(\mathcal{E})}$ is 2-times differentiable on $\mathcal{I} \supseteq \{x^{(\mathcal{E})}\}$ and, using the Taylor theorem at the point $x^{(\mathcal{E})}$, one obtains that

$$\mathrm{I}^{(\mathcal{E})}(x) = s(x^{(\mathcal{E})})\left(x - x^{(\mathcal{E})}\right) + \frac{1}{2}\partial_x s(x^{(\mathcal{E})})\left(x - x^{(\mathcal{E})}\right)^2 + o\left(\left(x - x^{(\mathcal{E})}\right)^2\right), \tag{5.26}$$

provided (5.23) holds true. Since, by (5.7), (5.22) and (5.25), $s(x^{(\mathcal{E})}) = 0$ and

$$\partial_x s(x^{(\mathcal{E})}) = \frac{1}{\partial_s f\,(0)} = \left.\frac{1}{\partial_s^2 \mathrm{J}^{(s\mathcal{E})}}\right|_{s=0},$$

one thus deduces (ii) from (5.26). ■

The behavior of the rate function within a neighborhood of the macroscopic current densities is directly related to the quantum fluctuations of the linear response current. Of course, one needs to ensure that $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} \neq 0$. If $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} = 0$, then it heuristically means that the convergence of the sequence $\{\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}\}_{L\in\mathbb{R}^+}$of microscopic current densities, in the KMS state $\varrho^{(\omega)}$ and with speed $|\Lambda_L|$, is in fact much faster than an exponential convergence. We do not expect this situation to appear in presence of disorders. We discuss this issue in Section 7.6 where we study sufficient conditions ensuring the strict positiveness of $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0}$. This study leads to the following theorem:

Theorem 5.4.2 (Sufficient conditions for non-zero quantum fluctuations)
Take ϑ, $\lambda, T \in \mathbb{R}_0^+$, $T, \beta \in \mathbb{R}^+ \in \mathbb{R}^+$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ with support in $[-T,0]$ and $\vec{w} \in \mathbb{R}^d$ with $\left\|\vec{w}\right\|_{\mathbb{R}^d} = 1$. Assume that the random variables $\{\omega_1(z)\}_{z\in\mathbb{Z}^d}$ are independently and identically distributed (i.i.d.). Then, for sufficiently small T and ϑ,

$$\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} \geq \frac{\lambda^2 \Upsilon^{(\mathcal{E},\vec{w})}}{(1+\mathrm{e}^{\beta(2d(2+\vartheta)+\lambda)})^2} \mathbb{E}\left[|\omega_1(0) - \mathbb{E}[\omega_1(0)]|^2\right]$$

with

$$\Upsilon^{(\mathcal{E},\vec{w})} \doteq \left(\int_{-\infty}^{0} \langle w, \mathcal{E}(\alpha)\rangle_{\mathbb{R}^d} \alpha^2 \mathrm{d}\alpha\right)^2 + \frac{1}{2}\sum_{k=1}^{d}\left(w_k \int_{-\infty}^{0} (\mathcal{E}(\alpha))_k \alpha^2 \mathrm{d}\alpha\right)^2 .$$

In particular, $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} \neq 0$ whenever $\Upsilon^{(\mathcal{E},\vec{w})} > 0$, $\mathbb{E}[|\omega_1(0) - \mathbb{E}[\omega_1(0)]|^2] > 0$ and T, ϑ are sufficiently small.

Proof: This is a direct consequence of a combination of (7.71) and (7.74) in Chapter 7. ■

Note that the fact that the random variables $\{\omega_1(z)\}_{z\in\mathbb{Z}^d}$ are independently and identically distributed (i.i.d.) is not essential here. In fact, by (7.68), (7.71) and (7.72), it suffices that

$$\mathbb{E}\left[\left|\int_{-\infty}^{0} \left\langle w^{(\omega)}, \mathcal{E}(\alpha)\right\rangle_{\mathbb{R}^d} \alpha^2 \mathrm{d}\alpha\right|^2\right] > 0$$

to ensure $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} \neq 0$, where, for any $\omega \in \Omega$, $w^{(\omega)} := (w_1^{(\omega)}, \ldots, w_d^{(\omega)}) \in \mathbb{R}^d$ is the random vector defined by

$$w_k^{(\omega)} := (2\omega_1(0) - \omega_1(e_k) - \omega_1(-e_k))\, w_k, \qquad k \in \{1,\ldots,d\}.$$

Theorem 5.4.2 can be applied to the celebrated tight-binding Anderson model, which corresponds to the special case $\vartheta = 0$. This is why we focus on this important example in this theorem. The remaining case of larger parameters $\vartheta, T \in \mathbb{R}_0^+$ can certainly be studied, but the argument would be more complicated and this is not done in this thesis.

Chapter 6

Classical KMS Condition from the Quantum Condition with the Bose-Hubbard Hamiltonian

This chapter is completely independent of the previous results on conductivity and heat transport properties, the notations may have changed. In particular, we treat the case of bosons. The creation/annihilation operators satisfy (3.7). The Kubo-Martin-Schwinger condition, see Definition 2.2.1, is a widely studied fundamental property in quantum statistical mechanics which characterises the thermal equilibrium states of quantum systems. Here, we prove that in a certain limiting regime of high temperature the classical KMS condition can be derived from the quantum condition in the simple case of the Bose-Hubbard dynamical system on a finite graph. The main ingredients of the proof are Golden-Thompson inequality, Bogoliubov inequality and semiclassical analysis.

6.1 General setup

A $\mathcal{W}^*-$ dynamical system $(\mathcal{A}, \tau_t)$ is a pair of a von Neumann algebra of observables $\mathcal{A}$ and a one-parameter group of automorphisms τ_t on $\mathcal{A}$, see Definition 1.2.5 as well as [26, Section 2.4.2] for the definition of a von Neumann algebra. Consider for instance a finite dimensional Hilbert space $\mathfrak{H}$ then $\mathcal{A}$ can be chosen to be the set of all operators $\mathcal{B}(\mathfrak{H})$ and τ_t to be the automorphism group defined by

$$\tau_t(A) = e^{itH} A\, e^{-itH}$$

for any $A \in \mathcal{A}$. The operator H denotes the Hamiltonian of a given quantum system and the couple $(\mathcal{A}, \tau_t)$ describes the dynamics. According to quantum statistical physics such system admits a unique thermal equilibrium state ω_β at inverse temperature β given by

$$\omega_\beta(A) = \frac{\operatorname{tr}(e^{-\beta H} A)}{\operatorname{tr}(e^{-\beta H})}, \quad A \in \mathcal{A}. \tag{6.1}$$

In general, the simplicity of the above statement has to be nuanced. In fact, the characterisation of thermal equilibrium in statistical mechanics is a nontrivial question particularly for dynamical systems which have an infinite number of degrees of freedom, see [27, 86]. One of the important and most elegant characterisation of equilibrium states was noticed by R. Kubo, P.C. Martin and J. Schwinger in the late fifties. It is based in the following observations in finite dimension. In fact, one remarks by a simple computation that the Gibbs state ω_β in (6.1) satisfies for all $t \in \mathbb{R}$ and any $A, B \in \mathcal{A}$ the identity,

$$\omega_\beta(A\ \tau_{t+i\beta}(B)) = \omega_\beta(\tau_t(B)A)\,, \tag{6.2}$$

where $\tau_{t+i\beta}(\cdot)$ denotes an analytic extension of the automorphism τ_t to complex times given by

$$\tau_{t+i\beta}(B) = e^{(-\beta+it)H} B\, e^{(\beta-it)H}\,.$$

More remarkable, if one takes a state ω that satisfies the same condition as (6.2) then ω should be the Gibbs state ω_β in (6.1). This indicates that the equation (6.2) singles out the thermal equilibrium states among all possible states of a quantum system. In the late sixties, R. Haag, N.M. Hugenholtz and M. Winnink suggested the identity (6.2) as a criterion for equilibrium states and they named it the KMS boundary condition after Kubo, Martin and Schwinger [79]. The subject of KMS states is by now deeply studied specially from an algebraic standpoint. For instance, various characterisations related to correlation inequalities and to variational principles have been derived (see e.g. [73, 68, 27]). Other perspectives have also been explored related for instance to the Tomita-Takasaki theory, the Heck algebra and number theory (see e.g. [71, 67, 69]).

In the seventies, G. Gallavotti and E. Verboven, suggested an analogue to the KMS boundary condition (6.2) which is suitable for classical mechanical systems and highlighted its relationship with the Kirkwood-Salzburg equations and with the Gibbs equilibrium measures, see [78]. The derivation of such condition is based in the following heuristic argument. Consider a state $\omega_\hbar$ satisfying the KMS boundary condition

$$\omega_\hbar\Big(BA\Big) = \omega_\hbar\Big(A\ \tau_{i\hbar\beta}(B)\Big) \tag{6.3}$$

at inverse temperature $\hbar\beta$, where $\hbar$ refers to the reduced Planck constant. This relation yields

$$\omega_\hbar\Big(\frac{AB-BA}{i\hbar}\Big) = \omega_\hbar\Big(A\ \frac{\tau_{i\hbar\beta}(B)-B}{i\hbar}\Big). \tag{6.4}$$

Assume for the moment that the space $\mathfrak{H} = L^2(\mathbb{R}^d)$, so one can consider that the Hamiltonian H and the observables A, B are given by $\hbar$-Weyl-quantized symbols (i.e., $H = h^{W,\hbar}$, $A = a^{W,\hbar}$ and $B = b^{W,\hbar}$ for some smooth functions a and b defined over the phase-space $\mathbb{R}^{2d}$). Then the semiclassical theory firstly tell us that

$$\frac{AB-BA}{i\hbar} \underset{\hbar\to 0}{\longrightarrow} \{a,b\}\,, \qquad \text{and} \qquad \frac{\tau_{i\hbar\beta}(B)-B}{i\hbar} \underset{\hbar\to 0}{\longrightarrow} \beta\,\{h,b\}\,, \tag{6.5}$$

where $\{\cdot,\cdot\}$ is a Poisson bracket and h denotes the Hamiltonian of the corresponding classical system. Secondly, the quantum states $\omega_\hbar$ (or at least a subsequence) converge in a weak sense to a semiclassical probability measure μ over $\mathbb{R}^{2d}$ when $\hbar \to 0$. Therefore, the expected classical KMS condition that should in principle characterise the statistical equilibrium for classical mechanical systems is formally given by

$$\mu\Big(\{a,b\}\Big) = \beta\,\mu\Big(a\,\{h,b\}\Big)\,, \tag{6.6}$$

for any smooth functions a, b on the phase-space $\mathbb{R}^{2d}$. Here the notation $\mu(f) = \int_{\mathbb{R}^{2d}} f(u)\,d\mu(u)$ is used. After the works [78, 63], M. Aizenman et al. showed in [64] that the condition (6.6) singles out thermal equilibrium states for infinite classical mechanical systems among all probability measures. In particular, the only measure μ satisfying (6.6) in our example is the Gibbs measure defined with respect to the Lebesgue measure by the density,

$$\mu_\beta = \frac{1}{z(\beta)}\,e^{-\beta h(u)}\,, \tag{6.7}$$

where $z(\beta)$ is a normalisation constant. Notice that the above Gibbs measure μ_β can also be characterised as an equilibrium state by means of variational methods and maximum entropy properties or by correlation inequalities, see [27]. Nevertheless, in this note we focus only in the KMS boundary conditions for classical and quantum systems. In general, the derivation of the classical KMS boundary condition (6.6) from the quantum one is a non trivial and interesting question which depends on the considered dynamical system. In our opinion, the classical KMS condition is an elegant characterisation of statistical equilibrium which deserves more attention from PDE analysts. Although this condition has been studied in some subsequent works (see e.g. [77, 83, 85, 84, 70, 74]), it seems not largely known.

Our main purpose in this section, is to provide a rigorous and simple proof for the derivation of the classical KMS condition (6.6) as a consequence of the relation (6.2) and the classical limit, $\hbar \to 0$, for the Bose-Hubbard dynamical system on a finite graph. The system we consider is governed by a typical many-body quantum Hamiltonian which can be written in terms of creation/annihilation operators and which is restricted to a finite volume. Our proof of convergence is based on the Golden-Thompson inequality, the Bogoliubov inequality and the semiclassical analysis in the Fock space. Since the classical phase-space of the system considered here is finite dimensional it is possible by change of representation to convert the problem to a semiclassical analysis in a L^2 space. However, we avoid such change since we lose most of the insight and most of the interesting structures of our problem. In particular, we will rely on the analysis on the phase-space given in [65]. Our interest in the Bose-Hubbard system is motivated by the establishment of a strong link between classical and quantum KMS conditions so that it leads to the exchange of the thermodynamic and the classical limits for infinite dynamical systems and to the investigation of phase transitions. Also note that from a physical standpoint the Bose-Hubbard model is a quite relevant model describing ultracold atoms in optical lattices with an observed phenomenon of superfluid-insulator transition. From a wider perspective, the question considered here is also related to the recent trend initiated by M. Lewin, P.T. Nam and N. Rougerie [81, 82] about the Gibbs measures for the nonlinear Schrödinger equations (see also [76] where these investigations were continued). In this respect, the KMS boundary conditions could provide an alternative proof for the convergence of Gibbs states. These questions will be considered elsewhere and here we will only focus on the Bose-Hubbard model on finite graph which is a much simpler model.

6.2 Quantum Hamiltonian on a finite graph

The discrete Laplacian: Consider a finite graph $G = (V, E)$ where V is the set of vertices and E is the set of edges. Assume furthermore that G is a simple undirected graph and let $\deg(x)$ denotes the degree of each vertices $x \in V$. In the following, we denote the graph equivalently G or V. Consider the Hilbert space of all complex-valued functions on V denoted as $\ell^2(G)$ and endowed with its natural scalar product and with the orthonormal basis $(e_x)_{x\in V}$ such that

$$e_x(y) := \delta_{x,y}, \quad \forall x, y \in V.$$

Then the discrete Laplacian on the graph G is a non-positive bounded operator on $\ell^2(G)$ given by

$$(\Delta_G \psi)(x) := -deg(x)\psi(x) + \sum_{y\in V, y\sim x} \psi(y),$$

with the above sum running over the nearest neighbours of x and ψ is any function in $\ell^2(G)$.

The Bose-Hubbard Hamiltonian: Consider the bosonic Fock space,

$$\mathfrak{F} = \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} \otimes_s^n \ell^2(G) \ ,$$

where $\otimes_s^n \ell^2(G)$ denotes the symmetric n-fold tensor product of $\ell^2(G)$. Compare with Equation (3.1) in Chapter 3. So, any $\psi \in \otimes_s^n \ell^2(G)$ is a functions $\psi : V^n \to \mathbb{C}$ invariant under any permutation of its variables. Introduce the usual creation/annihilation operators acting on the bosonic Fock space,

$$a_x = a(e_x) \quad \text{and} \quad a_x^* = a^*(e_x)\,,$$

then the following canonical commutation relations are satisfied,

$$\left[a_x, a_y^*\right] = \delta_{x,y}\, \mathbf{1}_{\mathfrak{F}} \quad \text{and} \quad \left[a_x^*, a_y^*\right] = \left[a_x, a_y\right] = 0, \quad \forall x, y \in V\,.$$

Compare with Equation (3.7) in Chapter 3.

Definition 6.2.1 (Bose-Hubbard Hamiltonian) *For $\varepsilon \in (0, \bar{\varepsilon})$, $\lambda > 0$ and $\kappa < 0$, define the ε-dependent Bose-Hubbard Hamiltonian on the bosonic Fock space $\mathfrak{F}$ by*

$$H_\varepsilon := \frac{\varepsilon}{2} \sum_{x,y \in V : y \sim x} (a_x^* - a_y^*)(a_x - a_y) + \frac{\varepsilon^2 \lambda}{2} \sum_{x \in V} a_x^* a_x^* a_x a_x - \varepsilon\kappa \sum_{x \in V} a_x^* a_x.$$

Here λ is the on-site interaction, κ is the chemical potential and ε is the semiclassical parameter.

Remark 6.2.2 *The first term of the Hamiltonian H_ε is the kinetic part of the system and corresponds to the second quantization of the discrete Laplacian. Indeed, one can write*

$$\frac{1}{2} \sum_{x,y \in V : y \sim x} (a_x^* - a_y^*)(a_x - a_y) = \sum_{x \in V} deg(x)\, a_x^* a_x - \sum_{x,y \in V, y \sim x} a_x^* a_y = \mathrm{d}\Gamma(-\Delta_G)\,,$$

where $\mathrm{d}\Gamma(\cdot)$ *is the second quantization operator defined on the bosonic Fock space by*

$$\mathrm{d}\Gamma(A)_{|\otimes_s^n \ell^2(G)} = \sum_{j=1}^{n} 1 \otimes \cdots \otimes A^{(j)} \otimes \cdots \otimes 1\,, \tag{6.8}$$

for any given operator $A \in \mathcal{B}(\ell^2(G))$ and where $A^{(j)}$ means that A acts only in the j-th component. See also Equation (3.10).

The following rescaled *number operator* will be often used,

$$N_\varepsilon := \varepsilon\, \mathrm{d}\Gamma(1_{\ell^2(G)}) = \varepsilon \sum_{x \in V} a_x^* a_x\,. \tag{6.9}$$

Therefore, one can rewrite the Bose-Hubbard Hamiltonian as follows

$$H_\varepsilon = \varepsilon\, \mathrm{d}\Gamma\Big(-\Delta_G - \kappa 1_{\ell^2(G)}\Big) + \varepsilon^2 \frac{\lambda}{2} I_G\,,$$

with the interaction denoted as

$$I_G := \sum_{x \in V} a_x^* a_x^* a_x a_x\,.$$

Since the discrete Laplacian Δ_G is self-adjoint, it is easy to check that H_ε defines an (unbounded) self-adjoint operator on the Fock space $\mathfrak{F}$ over its natural domain (for more details see e.g. [66, Appendix A]). Remark that the operator $-\Delta_G - \kappa 1_{\ell^2(G)}$ is positive since the chemical potential κ is negative.

6.3 Quantum KMS condition

The Bose-Hubbard Hamiltonian defines a $\mathcal{W}^*$ -dynamical system $(\mathfrak{M}, \alpha_t)$ where $\mathfrak{M}$ is the von Neumann algebra of all bounded operators $\mathcal{B}(\mathfrak{F})$ on the Fock space and α_t is the one parameter group of automorphisms defined by

$$\alpha_t(A) = e^{i\frac{t}{\varepsilon}H_\varepsilon} A\, e^{-i\frac{t}{\varepsilon}H_\varepsilon} ,$$

for any $A \in \mathfrak{M}$. The above group of automorphisms α_t admits a generator $S : \mathfrak{M} \to \mathfrak{M}$ with a domain

$$\mathcal{D}(S) = \{A \in \mathfrak{M},\ [H_\varepsilon, A] \in \mathfrak{M}\} ,$$

and satisfies for any $A \in \mathcal{D}(S)$,

$$S(A) = \lim_{t\to 0} \frac{\alpha_t(A) - A}{t} = \frac{i}{\varepsilon}[H_\varepsilon, A] .$$

The latter convergence is with respect to the σ-weak topology on $\mathfrak{M}$. Remark also that the dynamics α_t depend on the semiclassical parameter ε.

Next, we point out that the dynamical system $(\mathfrak{M}, \alpha_t)$ admits a unique KMS state at inverse temperature $\varepsilon\beta$. Here $\beta > 0$ is a fixed, ε-independent, effective inverse temperature.

Lemma 6.3.1 (Partition function)
Since the chemical potential κ is strictly negative then

$$\mathrm{tr}_{\mathfrak{F}}\left(e^{-\beta H_\varepsilon}\right) < \infty.$$

Proof: It is a consequence of [27, Proposition 5.2.27] and the Golden-Thompson inequality. The latter, see [75], says that for any Hermitian matrices A and B one has,

$$\mathrm{tr}\left(e^{A+B}\right) \leq \mathrm{tr}\left(e^{A}\, e^{B}\right) . \tag{6.10}$$

■

Definition 6.3.2 (Gibbs state)
The Gibbs equilibrium state of the Bose-Hubbard system on a finite graph is well defined and it is given by

$$\omega_\varepsilon(A) = \frac{\mathrm{tr}_{\mathfrak{F}}(e^{-\beta H_\varepsilon} A)}{\mathrm{tr}_{\mathfrak{F}}(e^{-\beta H_\varepsilon})} . \tag{6.11}$$

For the sake of completeness, we recall some useful details concerning the KMS states. One says that $A \in \mathfrak{M}$ is an *entire analytic element* of α_t if there exists a function $f : \mathbb{C} \to \mathfrak{M}$ such that $f(t) = \alpha_t(A)$ for all $t \in \mathbb{R}$ and such that for any trace-class operator $\rho \in \mathfrak{M}$ the function $z \in \mathbb{C} \to \mathrm{tr}(\rho f(z))$ is analytic. Let $\mathfrak{M}_\alpha$ denotes the set of entire analytic elements for α, then it is known that $\mathfrak{M}_\alpha$ is dense in $\mathfrak{M}$ with respect to the σ-weak topology. For more details on analytic elements, see [26, section 2.5.3]. In particular, by [26, Definition 2.5.20], an element $A \in \mathfrak{M}$ is entire analytic if and only if $A \in \mathcal{D}(S^n)$ for all $n \in \mathbb{N}$ and for any $t > 0$ the series below are absolutely convergent,

$$\sum_{n=0}^{\infty} \frac{t^n}{n!} \|S^n(A)\| < \infty \,. \tag{6.12}$$

Remark that on the set of entire analytic elements $\mathfrak{M}_\alpha$, the dynamics α_t can be extends to complex times. Indeed, $\alpha_z(A)$ is well defined, for any $A \in \mathfrak{M}_\alpha$, by the following absolutely convergent series,

$$\alpha_z(A) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \, S^n(A)\,, \quad \forall z \in \mathbb{C}\,.$$

We say that a state ω is a $(\alpha_t, \varepsilon\beta)$-KMS state if and only if ω is normal and for any $A, B \in \mathfrak{M}_\alpha$,

$$\omega(A \; \alpha_{i\varepsilon\beta}(B)) = \omega(BA)\,. \tag{6.13}$$

Remark that the above identity is known to be equivalent to the condition stated in the introduction (6.2). In particular, the KMS states are stationary states with respect to the dynamics.

Proposition 6.3.3 (Uniqueness of the KMS state)
The Gibbs state ω_ε defined by (6.11) *is the unique KMS state of the $\mathcal{W}^*$-dynamical system* $(\mathfrak{M}, \alpha_t)$ *at the inverse temperature $\varepsilon\beta$.*

Proof: For $B \in \mathfrak{M}_\alpha$, one checks

$$\alpha_{i\varepsilon\beta}(B) = e^{-\beta H_\varepsilon} B e^{\beta H_\varepsilon}\,.$$

Equation (6.11) for the Gibbs state gives

$$\omega_\varepsilon(A \; \alpha_{i\varepsilon\beta}(B)) = \frac{1}{\mathrm{tr}_{\mathfrak{F}}(e^{-\beta H_\varepsilon})} \mathrm{tr}_{\mathfrak{F}} \left(A \, e^{-\beta H_\varepsilon} B \right) = \omega_\varepsilon(BA)\,.$$

Reciprocally, let ω be a $(\alpha_t, \varepsilon\beta)$-KMS state. In particular, there exists a density matrix ρ such that $\mathrm{tr}_{\mathfrak{F}}(\rho) = 1$ and

$$\omega(A) = \mathrm{tr}_{\mathfrak{F}}(\rho \, A), \quad \forall A \in \mathfrak{M}\,.$$

Using the KMS condition (6.13) and the cyclicity of the trace, one proves for any $A \in \mathfrak{M}$,

$$\mathrm{tr}(\rho \, B \, A) = \mathrm{tr}(e^{-\beta H_\varepsilon} \, B \, e^{\beta H_\varepsilon} \rho \, A).$$

In particular, for any $B \in \mathfrak{M}_\alpha$,

$$\rho \, B = e^{-\beta H_\varepsilon} B \, e^{\beta H_\varepsilon} \rho\,. \tag{6.14}$$

Hence, one remarks that ρ commutes with any spectral projection of H_ε by taking for instance $B = 1_D(H_\varepsilon)$ in the equation (6.14). Therefore, one concludes that

$$e^{\beta H_\varepsilon}\,\rho\, B\,|_{1_D(H_\varepsilon)\mathfrak{F}} = B\, e^{\beta H_\varepsilon}\rho\,|_{1_D(H_\varepsilon)\mathfrak{F}}\ ,$$

for any bounded Borel subset D of $\mathbb{R}$ and any bounded operator B satisfying $B = 1_D(H_\varepsilon)B = B1_D(H_\varepsilon)$. So, the operator $e^{\beta H_\varepsilon}\,\rho$ commutes with any bounded operator over the subspaces $1_D(H_\varepsilon)\mathfrak{F}$. This implies that

$$\rho = c\, e^{-\beta H_\varepsilon}\ ,$$

and then one concludes with the fact that $\mathrm{tr}(\rho) = 1$. ■

6.4 Convergence

In this section, we prove that the KMS condition (6.13) converges, in the classical limit, towards the classical KMS condition. It is enough to prove such convergence for some specific observables $A, B \in \mathfrak{M}$. In fact, consider for $f, g \in \ell^2(G)$,

$$A = W(f)\,, \qquad \text{and} \qquad B = W(g)\,, \tag{6.15}$$

where $W(\cdot)$ denotes the Weyl operator defined by,

$$W(f) = e^{i\sqrt{\varepsilon}\,\Phi(f)}\,, \qquad \text{with} \quad \Phi(f) = \frac{a^*(f) + a(f)}{\sqrt{2}}\,. \tag{6.16}$$

Let $\chi \in C_0^\infty(\mathbb{R})$ such that $0 \le \chi \le 1$, $\chi \equiv 1$ if $|x| \le 1/2$ and $\chi \equiv 0$ if $|x| \ge 1$. Define, for $n \in \mathbb{N}$, the cut-off functions χ_n as

$$\chi_n(\cdot) = \chi\Big(\frac{\cdot}{n}\Big)\,.$$

Then, we are going to consider only the following smoothed observables,

$$A_n := \chi_n(N_\varepsilon)\, A\, \chi_n(N_\varepsilon)\,, \qquad \text{and} \qquad B_n := \chi_n(N_\varepsilon)\, B\, \chi_n(N_\varepsilon)\,. \tag{6.17}$$

Lemma 6.4.1 (Analytic elements)
For all $\varepsilon > 0$ and $n \in \mathbb{N}$, the elements A_n and B_n given by (6.17) *are entire analytic for the dynamics α_t.*

Proof: By functional calculus, remark that $1_{[0,n]}(N_\varepsilon)\chi_n(N_\varepsilon) = \chi_n(N_\varepsilon)$. Moreover, the number operator N_ε and the Hamiltonian H_ε commute in the strong sense. So, the generator S of the dynamics α_t satisfies for $k \in \mathbb{N}$,

$$\begin{aligned} S^k(A_n) &= \Big(\frac{i}{\varepsilon}\Big)^k\, [H_\varepsilon, \cdots [H_\varepsilon, A_n] \cdots]\,, \\ &= \Big(\frac{i}{\varepsilon}\Big)^k\, [\tilde{H}_\varepsilon, \cdots [\tilde{H}_\varepsilon, A_n] \cdots]\,, \end{aligned}$$

with $\tilde{H}_\varepsilon = 1_{[0,n]}(N_\varepsilon)H_\varepsilon$ being a bounded operator. Hence, the estimate (6.12) is satisfied and so A_n is a entire analytic element. ■

Recall that the $(\alpha_t, \varepsilon\beta)$-KMS state ω_ε satisfies in particular the condition

$$\omega_\varepsilon\left(A_n\,\alpha_{i\varepsilon\beta}(B_m)\right) = \omega_\varepsilon\left(B_m\,A_n\right)\,.$$

A simple computation then leads to the main identity

$$\omega_\varepsilon\left(A_n\,\frac{\alpha_{i\varepsilon\beta}(B_m) - B_m}{i\varepsilon}\right) = \omega_\varepsilon\left(\frac{[B_m, A_n]}{i\varepsilon}\right). \tag{6.18}$$

Our aim is to take the classical limit $\varepsilon \to 0$ in the above relation and to prove the convergence for the left- and right-hand sides so that we obtain the classical KMS boundary conditions. In order to take such a limit, one needs to use the semiclasscial (Wigner) measures of $\{\omega_\varepsilon\}_{\varepsilon\in(0,\bar{\varepsilon})}$. Recall that μ a Borel probability measure on the phase-space $\ell^2(G)$ is a Wigner measure of $\{\omega_\varepsilon\}_{\varepsilon\in(0,\bar{\varepsilon})}$ if there exists a subsequence $(\varepsilon_k)_{k\in\mathbb{N}}$ such that $\lim_{k\to\infty}\varepsilon_k = 0$ and for any $f \in \ell^2(G)$,

$$\lim_{k\to\infty}\omega_{\varepsilon_k}\left(W(f)\right) = \int_{\ell^2(G)} e^{i\sqrt{2}\Re\mathrm{e}\langle f,u\rangle}\,d\mu\,. \tag{6.19}$$

Note that the Weyl operator depends here on the parameter ε_k instead of ε as in (6.16). According to [65, Thm. 6.2] and Lemma 6.6.3, the family of KMS states $\{\omega_\varepsilon\}_{\varepsilon\in(0,\bar{\varepsilon})}$ admits a non-void set of Wigner probability measures. Later on, we will prove that this set of measures reduces to a singleton given by the Gibbs equilibrium measure. But for the moment, we will use subsequences as in the definition (6.19).

The classical Hamiltonian system related to the Bose-Hubbard model is given by the *Discrete Nonlinear Schrödinger* equation, see [80]. Its energy functional (or Hamiltonian) is given by

$$h(u) = -\langle u, \Delta_G\,u\rangle - \kappa\|u\|^2 + \frac{\lambda}{2}\sum_{j\in V}|u(j)|^4\,. \tag{6.20}$$

Notice that $\ell^2(G)$ is a complex Hilbert space and so in our framework the Poisson structure is defined as follows. For F, G smooth functions on $\ell^2(G)$, the Poisson bracket is given by

$$\{F, G\} := \frac{1}{i}\,\left(\partial_u F\cdot\partial_{\bar{u}}G - \partial_u G\cdot\partial_{\bar{u}}F\right)\,. \tag{6.21}$$

Here ∂_u and $\partial_{\bar{u}}$ are the standard differentiation with respect to u or $\bar{u}$.

Our main result is stated below.

Theorem 6.4.1 (Classical KMS condition)
Let ω_ε by the KMS state of the Bose-Hubbard $\mathcal{W}^*$-dynamical system $(\mathcal{A}, \alpha_t)$ at inverse temperature

$\varepsilon\beta$. Then any semiclassical (Wigner) measure of ω_ε satisfies the classical KMS condition, i.e., for any F, G smooth functions on $\ell^2(G)$,

$$\beta\;\mu(\{h,G\}\;F) = \mu(\{F,G\})\,, \tag{6.22}$$

where the classical Hamiltonian h is given by (6.20) *and $\{\cdot,\cdot\}$ denotes the Poisson bracket recalled in* (6.21).

In order to prove Theorem 6.4.1, one needs some preliminary steps.

Proposition 6.4.2 (Classical KMS condition - I)
Let $(\varepsilon_k)_{k\in\mathbb{N}}$ be a subsequence such that $\lim_{k\to\infty}\varepsilon_k = 0$. Assume that the family of KMS states $\{\omega_{\varepsilon_k}\}_{k\in\mathbb{N}}$ admits a unique Wigner measure μ. Then for all n, m integers such that $m \geq 2n$,

$$\lim_{k\to\infty}\omega_{\varepsilon_k}\left(\frac{[B_m, A_n]}{i\varepsilon_k}\right) = \int_{\ell^2(G)} \chi_n^2(\langle u,u\rangle)\;\{e^{\sqrt{2}i\Re\mathrm{e}\langle g,u\rangle}; e^{\sqrt{2}i\Re\mathrm{e}\langle f,u\rangle}\}\;d\mu \tag{6.23}$$

$$+\int_{\ell^2(G)} \chi_n(\langle u,u\rangle)\;\{e^{\sqrt{2}i\Re\mathrm{e}\langle g,u\rangle}; \chi_n(\langle u,u\rangle)\}\;e^{\sqrt{2}i\Re\mathrm{e}\langle f,u\rangle}\;d\mu \tag{6.24}$$

$$+\int_{\ell^2(G)} \chi_n(\langle u,u\rangle)\;\{\chi_n(\langle u,u\rangle); e^{\sqrt{2}i\Re\mathrm{e}\langle f,u\rangle}\}\;e^{\sqrt{2}i\Re\mathrm{e}\langle g,u\rangle}\;d\mu\,. \tag{6.25}$$

Proof: For simplicity, we denote ε instead of ε_k and χ_m instead of $\chi_m(N_\varepsilon)$. Using the cyclicity of the trace and the fact that $\chi_n\chi_m = \chi_n$ ($m \geq 2n$), one remarks that

$$\omega_\varepsilon\left([B_m, A_n]\right) = \omega_\varepsilon\left(\chi_n\left(B\chi_n A - A\chi_n B\right)\right)\,.$$

A simple computation yields

$$\begin{aligned}\lim_{\varepsilon\to0}\omega_\varepsilon\left(\frac{[B_m, A_n]}{i\varepsilon}\right) &= \lim_{\varepsilon\to0}\omega_\varepsilon\left(\chi_n^2\,\frac{[B,A]}{i\varepsilon}\right)\\ &+ \lim_{\varepsilon\to0}\omega_\varepsilon\left(\chi_n\,\frac{[B,\chi_n]}{i\varepsilon}\,A\right)\\ &+ \lim_{\varepsilon\to0}\omega_\varepsilon\left(\chi_n\,\frac{[\chi_n,A]}{i\varepsilon}\,B\right)\,.\end{aligned} \tag{6.26}$$

The Weyl commutation relations gives

$$\frac{[B,A]}{i\varepsilon} = W(f+g)\;(\Im\mathrm{m}\langle f,g\rangle + O(\varepsilon))\,.$$

So, using [65, Thm. 6.13],

$$\begin{aligned}\lim_{\varepsilon\to0}\omega_\varepsilon\left(\chi_n^2\,\frac{[B,A]}{i\varepsilon}\right) &= \Im\mathrm{m}\langle f,g\rangle\;\lim_{\varepsilon\to0}\omega_\varepsilon\left(\chi_n^2\,W(f+g)\right)\\ &= \Im\mathrm{m}\langle f,g\rangle\int_{\ell^2(G)}\chi_n^2(\langle u,u\rangle)\;e^{\sqrt{2}i\Re\mathrm{e}\langle f+g,u\rangle}\;d\mu\,.\end{aligned}$$

Checking the Poisson bracket,

$$\{e^{\sqrt{2}i\Re\mathrm{e}\langle g,u\rangle}; e^{\sqrt{2}i\Re\mathrm{e}\langle f,u\rangle}\} = \Im\mathrm{m}\langle f,g\rangle\, e^{\sqrt{2}i\Re\mathrm{e}\langle f+g,u\rangle},$$

one obtains the right-hand side of (6.23). Consider now the second term in (6.26). One can write

$$[W(g),\chi_n] = \int_{\mathbb{R}} \hat{\chi}_n(s)\,[W(g),e^{isN_\varepsilon}]\,\frac{ds}{\sqrt{2\pi}},$$

where $\hat{\chi}_n$ denotes the Fourier transform of the function $\chi_n(\cdot)$. Using standard computations in the Fock space and Taylor expansion,

$$\begin{aligned}
\left[W(g),\mathrm{e}^{isN_\varepsilon}\right] &= \mathrm{e}^{isN_\varepsilon}\left(\mathrm{e}^{-isN_\varepsilon}W(g)\mathrm{e}^{isN_\varepsilon} - W(g)\right)\\
&= i\mathrm{e}^{isN_\varepsilon}\int_0^s \mathrm{e}^{-irN_\varepsilon}[W(g),N_\varepsilon]\,\mathrm{e}^{irN_\varepsilon}\,dr\\
&= -\,\mathrm{e}^{isN_\varepsilon}\int_0^s \mathrm{e}^{-irN_\varepsilon}W(g)\left(\varepsilon\Phi(ig)+\frac{\varepsilon^2}{2}\|g\|^2\right)\mathrm{e}^{irN_\varepsilon}\,dr.
\end{aligned}$$

Hence, using the cyclicity of the trace

$$\lim_{\varepsilon\to0}\omega_\varepsilon\left(\chi_n\,\frac{[B,\chi_n]}{i\varepsilon}\,A\right) = -\int_{\mathbb{R}} s\hat{\chi}_n(s)\,\lim_{\varepsilon\to0}\omega_\varepsilon\left(\chi_n\,e^{isN_\varepsilon}W(g)\Phi(ig)W(f)\right)\,\frac{ds}{\sqrt{2\pi}}. \tag{6.27}$$

Knowing, by Lemma 6.7.1, that the Wigner measure of the sequence $\{W(f)\rho_\varepsilon\chi_n(N_\varepsilon)e^{isN_\varepsilon}W(g)\}$ is given by

$$\left\{\mu\chi_n(\langle u,u\rangle)e^{is\|u\|^2}e^{\sqrt{2}i\Re\mathrm{e}\langle g+f,u\rangle}\right\},$$

then one obtains using [65, Thm. 6.13],

$$\lim_{\varepsilon\to0}\omega_\varepsilon\left(\chi_n\,\frac{[B,\chi_n]}{i\varepsilon}\,A\right) = -\sqrt{2}\int_{\mathbb{R}} s\hat{\chi}_n(s)\int_{\ell^2(G)}\chi_n(\langle u,u\rangle)\,e^{is\|u\|^2}\,\Re\mathrm{e}\langle u,ig\rangle e^{\sqrt{2}i\Re\mathrm{e}\langle g+f,u\rangle}d\mu\,\frac{ds}{\sqrt{2\pi}}.$$

Integrating back with respect to the variable s,

$$\lim_{\varepsilon\to0}\omega_\varepsilon\left(\chi_n\,\frac{[B,\chi_n]}{i\varepsilon}\,A\right) = \sqrt{2}i\int_{\ell^2(G)}\chi_n'(\|u\|^2)\,\chi_n(\|u\|^2)\,\Im\mathrm{m}\langle g,u\rangle e^{\sqrt{2}i\Re\mathrm{e}\langle g+f,u\rangle}\,d\mu.$$

Then checking the Poisson bracket

$$\left\{e^{\sqrt{2}i\Re\mathrm{e}\langle g,u\rangle};\chi_n(\langle u,u\rangle)\right\} = \sqrt{2}i\chi_n'(\|u\|^2)\,\Im\mathrm{m}\langle g,u\rangle e^{\sqrt{2}i\Re\mathrm{e}\langle g,u\rangle},$$

yields the right-hand side of (6.24). The third term in the right side of (6.26) is similar to the above one. ■

The next step is to prove the convergence of the right hand side of (6.18).

Lemma 6.4.3 (Classical KMS condition - II)
Let $(\varepsilon_k)_{k\in\mathbb{N}}$ be a subsequence such that $\lim_{k\to\infty}\varepsilon_k = 0$. Assume that the family of KMS states $\{\omega_{\varepsilon_k}\}_{k\in\mathbb{N}}$ admits a unique Wigner measure μ. Then for all n, m integers such that $m \geq 2n$,

$$\lim_{k\to\infty}\omega_{\varepsilon_k}\left(A_n\,\frac{\alpha_{i\varepsilon_k\beta}(B_m)-B_m}{i\varepsilon_k}\right)=\beta\,\lim_{k\to\infty}\omega_{\varepsilon_k}\left(A_n\,\frac{[B_m,H_{\varepsilon_k}]}{i\varepsilon_k}\right). \tag{6.28}$$

Proof: For simplicity, we use ε instead of ε_k. According to Lemma 6.4.1, B_m is a entire analytic element for the dynamics α_t. Hence, by Taylor expansion,

$$\omega_\varepsilon\left(A_n\,\frac{\alpha_{i\varepsilon\beta}(B_m)-B_m}{i\varepsilon}\right)=\beta\int_0^1\omega_\varepsilon\left(A_n\frac{[\alpha_{is\varepsilon\beta}(B_m),H_\varepsilon]}{i\varepsilon}\right)\,ds\,.$$

Using the cyclicity of the trace and the fact that A_n, B_m are entire analytic elements,

$$\omega_\varepsilon\left(A_n\frac{[\alpha_{is\varepsilon\beta}(B_m),H_\varepsilon]}{i\varepsilon}\right)=\omega_\varepsilon\left(e^{s\beta H_\varepsilon}\,A_n\,e^{-s\beta H_\varepsilon}\,\frac{[B_m,H_\varepsilon]}{i\varepsilon}\right).$$

A second Taylor expansion yields,

$$\begin{aligned}\omega_\varepsilon\left(A_n\,\frac{[\alpha_{is\varepsilon\beta}(B_m),H_\varepsilon]}{i\varepsilon}\right)&=\omega_\varepsilon\left(A_n\,\frac{[B_m,H_\varepsilon]}{i\varepsilon}\right)\\&\quad+\beta\int_0^s\omega_\varepsilon\left(e^{r\beta H_\varepsilon}\,[H_\varepsilon,A_n]\,e^{-r\beta H_\varepsilon}\,\frac{[B_m,H_\varepsilon]}{i\varepsilon}\right)dr\,.\end{aligned}$$

So, the equality (6.28) is proved since

$$\lim_{\varepsilon\to0}\int_0^1 ds\int_0^s dr\;\;\omega_\varepsilon\left([H_\varepsilon,\alpha_{-is\varepsilon\beta}(A_n)]\;\frac{[B_m,H_\varepsilon]}{i\varepsilon}\right)=0\,,$$

thanks to the Lemma 6.7.2. ■

Proposition 6.4.4 (Classical KMS condition - III)
Let $(\varepsilon_k)_{k\in\mathbb{N}}$ be a subsequence such that $\lim_{k\to\infty}\varepsilon_k = 0$. Assume that the family of KMS states $\{\omega_{\varepsilon_k}\}_{k\in\mathbb{N}}$ admits a unique Wigner measure μ. Then for all n, m integers such that $m \geq 2n$,

$$\lim_{k\to\infty}\omega_{\varepsilon_k}\left(A_n\,\frac{\alpha_{i\varepsilon\beta}(B_m)-B_m}{i\varepsilon}\right)=\beta\int_{\ell^2(G)}\chi_n^2(\langle u,u\rangle)\;\{e^{\sqrt{2}i\Re\mathrm{e}\langle g,u\rangle};h(u)\}\,e^{\sqrt{2}i\Re\mathrm{e}\langle f,u\rangle}\;d\mu\,. \tag{6.29}$$

Proof: The previous Lemma 6.4.3 allowed to get rid of the dynamics at complex times. So, it is enough to show the limit,

$$\lim_{k\to\infty}\omega_{\varepsilon_k}\left(A_n\,\frac{[B_m,H_{\varepsilon_k}]}{i\varepsilon_k}\right)=\int_{\ell^2(G)}\chi_n^2(\langle u,u\rangle)\;\{e^{\sqrt{2}i\Re\mathrm{e}\langle g,u\rangle};h(u)\}\,e^{\sqrt{2}i\Re\mathrm{e}\langle f,u\rangle}\;d\mu\,.$$

For simplicity, we denote ε instead of ε_k and χ_m instead of $\chi_m(N_\varepsilon)$. Since $m \geq 2n$ then $\chi_n\chi_m = \chi_n$ and one notices that

$$\chi_n A\chi_n\,[\chi_m B\chi_m, H_\varepsilon] = \chi_n A\chi_n\,[B, H_\varepsilon]\,\chi_m = \chi_n A\chi_n\,[W(g), H_\varepsilon]\,\chi_m\,.$$

Standard computations on the Fock space yield, (see e.g. [65, Proposition 2.10]),

$$\begin{aligned}\frac{i}{\varepsilon}[B, H_\varepsilon] &= \frac{i}{\varepsilon}\left(W(g)H_\varepsilon W(g)^* - H\right)\, W(g)\\ &= \frac{i}{\varepsilon}\left(h(\cdot - \frac{i\varepsilon}{\sqrt{2}}g) - h(u)\right)^{Wick}\, W(g)\\ &= \left(\underbrace{\{\sqrt{2}\,\Re\mathrm{e}\langle g, u\rangle, h(u)\}^{Wick}}_{C^{Wick}} + R(\varepsilon)^{Wick}\right)\, W(g)\,.\end{aligned}$$

The subscript *Wick* refers to the Wick quantization, see [65, section 2]. The remainder $R(\varepsilon)^{Wick}$ can be explicitly computed and satisfies the uniform estimate

$$\|\chi_n(N_\varepsilon)\; R(\varepsilon)^{Wick}\| \leq c\;\varepsilon\,,$$

which can be easily proved using [65, Lemma 2.5]. Therefore using Lemma 6.7.2, one shows

$$\begin{aligned}\lim_{k\to\infty}\omega_{\varepsilon_k}\left(A_n\,\frac{\alpha_{i\varepsilon\beta}(B_m) - B_m}{i\varepsilon}\right) &= \beta\lim_{k\to\infty}\omega_{\varepsilon_k}\left(\chi_n A\chi_n\, C^{Wick}B\right)\\ &= \beta\lim_{k\to\infty}\omega_{\varepsilon_k}\left(\chi_n^2 A\, C^{Wick}B\right)\,.\end{aligned}$$

Knowing, by Lemma 6.7.1, that the Wigner measure of the sequence $\{W(g)\rho_\varepsilon\chi_n^2(N_\varepsilon)W(f)\}$ is given by

$$\left\{\mu e^{\sqrt{2}i\Re\mathrm{e}\langle f+g,u\rangle}\chi_n^2(\|u\|^2)\right\},$$

one concludes by [65, Thm. 6.13],

$$\lim_{\varepsilon\to 0}\omega_\varepsilon\left(A_n\,\frac{\alpha_{i\varepsilon\beta}(B_m) - B_m}{i\varepsilon}\right) = \int_{\ell^2(G)}\chi_n^2(\|u\|^2)\; e^{\sqrt{2}i\Re\mathrm{e}\langle f+g,u\rangle}C(u)\; d\mu\,.$$

■

Corollary 6.4.5 *Any Wigner measure of the $(\alpha_t, \varepsilon\beta)$-KMS family of states ω_ε satisfies for all $f, g \in \ell^2(G)$,*

$$\beta\,\int_{\ell^2(G)}\{e^{i\Re\mathrm{e}\langle g,u\rangle}; h(u)\}\, e^{i\Re\mathrm{e}\langle f,u\rangle}\; d\mu \;=\; \int_{\ell^2(G)}\{e^{i\Re\mathrm{e}\langle g,u\rangle}; e^{i\Re\mathrm{e}\langle f,u\rangle}\}\; d\mu\,. \tag{6.30}$$

Proof: It is a consequence of Proposition 6.4.2, Proposition 6.4.4 and dominated convergence while taking $n, m \to \infty$. ■

Thus, we come to the following conclusion.

Proof: [Proof of Theorem 6.4.1] The phase-space $\ell^2(G)$ is a euclidean space. Let F, G be two smooth functions in $C_0^\infty(\ell^2(G))$. The inverse Fourier transform gives,

$$F(u) = \int_{\ell^2(G)} e^{i\Re e\langle f,u\rangle}\,\hat{F}(f)\,dL(f)\,, \qquad \text{and} \qquad G(u) = \int_{\ell^2(G)} e^{i\Re e\langle g,u\rangle}\,\hat{G}(g)\,dL(g)\,,$$

where $\hat{F}, \hat{G}$ denote the Fourier transforms of F and G respectively. Multiplying the equation (6.30) by $\hat{F}(f)\hat{G}(g)$ and integrating with respect to the Lebesgue measure in the variables f and g, one obtains

$$\beta \int_{\ell^2(G)} \{G(u), h(u)\}\, F(u)\, d\mu \;=\; \int_{\ell^2(G)} \{G(u), F(u)\}\, d\mu\,.$$

This proves the classical KMS condition (6.22). ■

6.5 Classical KMS condition

In this section, we point out that the only probability measure satisfying the classical KMS condition is the Gibbs equilibrium measure. This is a known fact and we provide here a short proof only for reader's convenience. The argument used below is borrowed from the work of M. Aizenman, S. Goldstein, C. Grubber, J. Lebowitz and P.A. Martin [64].

Proposition 6.5.1 (Gibbs measure) *Suppose that μ is a Borel probability measure on $\ell^2(G)$ satisfying the classical KMS condition* (6.22). *Then μ is the Gibbs equilibrium measure, i.e.,*

$$\frac{d\mu}{dL} = \frac{e^{-\beta\, h(u)}}{z(\beta)}\,, \qquad \textit{and} \qquad z(\beta) = \int_{\ell^2(G)} e^{-\beta\, h(u)}\, dL(u)\,,$$

with $h(\cdot)$ is the classical Hamiltonian of the DNLS equation given by (6.20) *and dL is the Lebesgue measure on $\ell^2(G)$.*

Proof: Consider the Borel probability measure $\nu = e^{\beta h(u)}\mu$, so that for any Borel set $\mathcal{B}$,

$$\nu(\mathcal{B}) = \int_{\mathcal{B}} e^{\beta h(u)} d\mu\,.$$

Notice that, for any $F, G \in C_0^\infty(\ell^2(G))$, the Poisson bracket satisfies

$$\Big\{F e^{-\beta h(u)}, G\Big\} = \Big\{F, G\Big\}\, e^{-\beta h(u)} - \beta \Big\{h, G\Big\}\, F(u) e^{-\beta h(u)}\,.$$

Hence, the classical KMS condition (6.22) can be written as

$$\mu\left(e^{\beta h(u)}\Big\{Fe^{-\beta h(u)}, G\Big\}\right) = 0\,,$$

or equivalently for any $F, G \in C_0^\infty(\ell^2(G))$,

$$\nu\left(\Big\{Fe^{-\beta h(u)}, G\Big\}\right) = 0\,.$$

Remark that the classical Hamiltonian h is a smooth $C_0^\infty(\ell^2(G))$. Hence, the measure ν satisfies for any $F, G \in C_0^\infty(\ell^2(G))$,

$$\nu\left(\Big\{F, G\Big\}\right) = 0\,.$$

This condition implies that ν is a multiple of the Lebesgue measure. Indeed, take $g(\cdot) = \langle e_j, \cdot\rangle\, \varphi(\cdot)$ with $\varphi \in C_0^\infty(\ell^2(G))$ being equal to 1 on the support of f. Then the Poisson bracket gives,

$$\{f, g\} = -i\partial_j f\,.$$

So, in a distributional sense the derivatives of the measure ν is null and therefore $d\nu = c\, dL$ for some constant c. Using the normalisation requirement for μ, one concludes that $d\nu = \frac{1}{z(\beta)}\, dL$. ■

6.6 Number estimates

Consider the quasi-free state $\omega_\varepsilon^0(\cdot)$ given by

$$\omega_\varepsilon^0(\cdot) = \frac{\mathrm{tr}\left(\cdot\;\; e^{\beta\varepsilon \mathrm{d}\Gamma(\Delta_G + \kappa 1)}\right)}{\mathrm{tr}\left(e^{\beta\varepsilon \mathrm{d}\Gamma(\Delta_G + \kappa 1)}\right)}\,.$$

The following uniform number of particles estimates are well know. Here we recall them for reader's convenience. For more details on quasi-free states and such inequalities, see e.g. [27, 81, 76]. Remember that the rescaled number operator is given by,

$$N_\varepsilon := \mathrm{d}\Gamma\left(1_{\ell^2(G)}\right) = \varepsilon \sum_{x \in V} a_x^* a_x.$$

Lemma 6.6.1 *For any $k \in \mathbb{N}$, there exists a positive constant c_k such that*

$$\omega_\varepsilon^0(N_\varepsilon^k) \leq c_k\,,$$

uniformly with respect to $\varepsilon \in (0, \bar{\varepsilon})$.

Proof: Recall that

$$N_\varepsilon := \varepsilon \sum_{x\in V} a_x^* a_x.$$

By using the quasi-free property of ω_ε^0, one has

$$\omega_\varepsilon^0(a_x^* a_x) = \langle e_x, \left(\frac{1}{e^{\beta\varepsilon(\Delta_G+\kappa 1)}-1}\right) e_x\rangle_{\ell^2(\mathcal{G})}.$$

Therefore, the following inequality holds true

$$\omega_\varepsilon^0(N_\varepsilon) \leq \varepsilon \operatorname{tr}\left(\frac{1}{e^{\beta\varepsilon(\Delta_G+\kappa 1)}-1}\right).$$

For $\varepsilon \in (0, \bar{\varepsilon})$, one has

$$e^{\beta\varepsilon(\Delta_G+\kappa 1)} - 1 = \beta\varepsilon(\Delta_G + \kappa 1) + O(\varepsilon^2). \tag{6.31}$$

This concludes the proof for $k = 1$. Now, for $k \geq 1$, observe that for any $x, y \in G$

$$\begin{aligned}\sum_{x,y\in G} \omega_\varepsilon^0(a_x^* a_y)\omega_\varepsilon^0(a_y^* a_x) &= \sum_{x,y\in G} \langle e_y, \left(\frac{1}{e^{\beta\varepsilon(\Delta_G+\kappa 1)}-1}\right) e_x\rangle_{\ell^2(\mathcal{G})} \langle e_x, \left(\frac{1}{e^{\beta\varepsilon(\Delta_G+\kappa 1)}-1}\right) e_y\rangle_{\ell^2(\mathcal{G})} \\ &= \sum_{y\in G} \langle e_y, \left(\frac{1}{e^{\beta\varepsilon(\Delta_G+\kappa 1)}-1}\right) P_G \left(\frac{1}{e^{\beta\varepsilon(\Delta_G+\kappa 1)}-1}\right) e_y\rangle_{\ell^2(\mathcal{G})} \\ &= \operatorname{tr}\left(\left(\frac{1}{e^{\beta\varepsilon(\Delta_G+\kappa 1)}-1}\right) P_G \left(\frac{1}{e^{\beta\varepsilon(\Delta_G+\kappa 1)}-1}\right)\right)\end{aligned}$$

where P_G is the orthogonal projection within the graph G. By using the same trick as above (see (6.31)), one obtains a term that is $O(\varepsilon^2)$. For $k > 1$,

$$\omega_\varepsilon^0(N_\varepsilon^k) = \varepsilon^k \sum_{x_1 \dots x_k \in G} \omega_\varepsilon^0(a_{x_1}^* a_{x_1} \dots a_{x_k}^* a_{x_k}).$$

Since ω_ε^0 is a quasi-free state and by using the canonical commutational relations $\omega_\varepsilon^0(a_{x_1}^* a_{x_1} \dots a_{x_k}^* a_{x_k})$ equals to a k-products + $(k-1)$-products + ... of

$$\omega_\varepsilon^0(a_{x_i}^* a_{x_j}), \quad 1 \leq i, j \leq k.$$

This implies that in order to control $\omega_\varepsilon^0(N_\varepsilon^k)$, $k \geq 1$, one needs an estimate on

$$\sum_{p=0}^{k} \operatorname{tr}\left(\underbrace{\left(\frac{1}{e^{\beta\varepsilon(\Delta_G+\kappa 1)}-1}\right) P_G \dots P_G \left(\frac{1}{e^{\beta\varepsilon(\Delta_G+\kappa 1)}-1}\right)}_{k-p \text{ terms } \frac{1}{e^{\beta\varepsilon(\Delta_G+\kappa 1)}-1}}\right) \operatorname{tr}\left(\frac{1}{e^{\beta\varepsilon(\Delta_G+\kappa 1)}-1}\right)^p$$

Once again, by using a same trick as in (6.31), one obtains a term that is $O(\varepsilon^k)$. ∎

Lemma 6.6.2 *There exists a positive constant c such that*

$$\frac{\mathrm{tr}(e^{\beta\varepsilon \mathrm{d}\Gamma(\Delta_G+\kappa 1)})}{\mathrm{tr}(e^{-\beta H_\varepsilon})} \leq c\,,$$

uniformly with respect to $\varepsilon \in (0, \bar{\varepsilon})$.

Proof: By using a Bogoliubov type inequality, see [87, Appendix D], one has that

$$\ln(\mathrm{tr}(e^{\beta\varepsilon \mathrm{d}\Gamma(\Delta_G+\kappa 1)})) - \ln(\mathrm{tr}(e^{-\beta H_\varepsilon})) \leq \beta\, \frac{\mathrm{tr}\left(\left(\varepsilon^2\, \frac{\lambda}{2} I_G - \kappa N_\varepsilon\right) e^{\beta\varepsilon \mathrm{d}\Gamma(\Delta_G+\kappa 1)}\right)}{\mathrm{tr}\left(e^{\beta\varepsilon \mathrm{d}\Gamma(\Delta_G+\kappa 1)}\right)}.$$

According to Definition 6.2.1, recall that

$$I_G = \sum_{x \in V} a_x^* a_x^* a_x a_x\,.$$

Therefore, there exists $c > 0$ such that

$$\ln(\mathrm{tr}(e^{\beta\varepsilon \mathrm{d}\Gamma(\Delta_G+\kappa 1)})) - \ln(\mathrm{tr}(e^{-\beta H^\varepsilon})) \leq c\left(\omega_\varepsilon^0(N_\varepsilon^2) + \omega_\varepsilon^0(N_\varepsilon)\right).$$

Using Lemma 6.6.1, one proves the inequality. ■

Lemma 6.6.3 *For any* $k \in \mathbb{N}$*, there exists a positive constant* c_k *such that*

$$\omega_\varepsilon(N_\varepsilon^k) \leq c_k\,,$$

uniformly with respect to $\varepsilon \in (0, \bar{\varepsilon})$.

Proof: A direct consequence of Lemma 6.6.1, Lemma 6.6.2 and the Golden-Thompson inequality. ■

6.7 Technical estimates

We refer the reader to [65] for more details in the semiclassical analysis on the Fock space. Here, we only sketch some useful technical results based in the above work. Remember that the KMS states ω_ε, given by (6.11), are normal and so we denote,

$$\omega_\varepsilon(\cdot) = \mathrm{tr}_{\mathfrak{F}}\left(\rho_\varepsilon\, \cdot\right).$$

Furthermore, assume for a subsequence $(\varepsilon_k)_{k\in\mathbb{N}}$, such that $\lim_{k\to\infty} \varepsilon_k = 0$, that the set $\{\rho_{\varepsilon_k}\}_{k\in\mathbb{N}}$ admits a unique Wigner measure μ. Then the following result holds true.

Lemma 6.7.1 *For any $\chi \in C_0^\infty(\mathbb{R})$ and $f, g \in \ell^2(G)$, the set $\{W(f)\rho_{\varepsilon_k}\chi(N_{\varepsilon_k})W(g)\}_{k\in\mathbb{N}}$ admits a unique Wigner measure given by*

$$\left\{\mu\, e^{\sqrt{2}i\Re\mathrm{e}\langle f+g,u\rangle}\chi(\|u\|^2)\right\}.$$

Proof: For simplicity, we denote ε instead of ε_k. It is enough to prove that the set of Wigner measures for the density matrices $\{\rho_\varepsilon\chi(N_\varepsilon)\}$ is the singleton

$$\{\mu\ \chi(\|u\|^2)\}.$$

In fact, using the Weyl commutation relations, one checks according to (6.19),

$$\lim_{\varepsilon\to 0}\mathrm{tr}_{\mathfrak{F}}\left(W(f)\rho_\varepsilon\chi(N_\varepsilon)W(g)\ W(\eta)\right) = \int_{\ell^2(G)} e^{i\sqrt{2}\Re\mathrm{e}\langle f+g+\eta,u\rangle}\, d\nu\,,$$

where ν is a Wigner measure of the set of density matrices $\{\rho_\varepsilon\chi(N_\varepsilon)\}$ (modulo subsequences). Now, using Pseudo-differential calculus,

$$\chi(N_\varepsilon) = \left(\chi(\|u\|^2)\right)^{Weyl} + O(\varepsilon)\,,$$

where the subscript refers to the Weyl ε-quantization and the difference between the right and left operator is of order ε in norm (see e.g. [72, Thm. 8.7]). Then [65, Thm. 6.13] with Lemma 6.6.3, gives

$$\nu = \mu\ \chi(\|u\|^2)\,.$$

■

Lemma 6.7.2 *For any $\chi \in C_0^\infty(\mathbb{R})$ and $f \in \ell^2(G)$, there exists $c > 0$ such that for all $\varepsilon \in (0, \bar{\varepsilon})$,*

$$\|\chi(N_\varepsilon)\,[N_\varepsilon, W(f)]\ \chi(N_\varepsilon)\| \le c\ \varepsilon\,, \qquad \textit{and} \qquad \|\chi(N_\varepsilon)\,[H_\varepsilon, W(f)]\ \chi(N_\varepsilon)\| \le c\ \varepsilon\,.$$

Proof: The proof of the two inequalities are similar. We sketch the second one. Using standard computation in the Fock space (see e.g. [65, Proposition 2.10]),

$$[H_\varepsilon, W(f)] = W(f)\ \left(h(\cdot + i\frac{\varepsilon}{\sqrt{2}}f) - h(u)\right)^{Wick}\,,$$

where the subscript refers to the Wick quantization, see [65, Section 2], and h is the classical Hamiltonian in (6.20). By Taylor expansion, one writes

$$h(\cdot + i\frac{\varepsilon}{\sqrt{2}}f) - h(u) = \varepsilon\, C_\varepsilon(u)\,, \tag{6.32}$$

where $C_\varepsilon(u)$ is a polynomial in u which can be computed explicitly. Using the number estimate in [65, Lemma 2.5], one proves the inequality. ■

Chapter 7

Technical proofs

7.1 Preliminary Definitions

Following the space restriction that we apply in the lattice, let us introduce the following sets:

$$\mathfrak{Z} := \left\{ \mathcal{Z} \in 2^{\mathbb{Z}^d} : \ (\forall Z_1, Z_2 \in \mathcal{Z}) \ Z_1 \neq Z_2 \Longrightarrow Z_1 \cap Z_2 = \emptyset \right\},$$
$$\mathfrak{Z}_{\mathrm{f}} := \{ \mathcal{Z} \in \mathfrak{Z} : \ |\mathcal{Z}| < \infty \text{ and } (\forall Z \in \mathcal{Z}) \ 0 < |Z| < \infty \}.$$

Those sets will appear to be very useful in the technical proofs. Observe that the one particle Hamiltonian within $\mathcal{Z} \in \mathfrak{Z}$ is given by

$$h_{\mathcal{Z}}^{(\omega)} := \sum_{Z \in \mathcal{Z}} P_Z h^{(\omega)} P_Z.$$

P_Z being the orthogonal projection within the subset Z of the lattice, see (4.9).

7.2 Preliminary estimates

We start by giving three general estimates which will be used many times afterwards. The first estimates are some elementary observations:

Lemma 7.2.1 (Operator norm estimate-I)
For any $C \in \mathcal{B}(\mathfrak{h})$*,*

$$\|C\|_{\mathcal{B}(\mathfrak{h})} = \sup_{\varphi, \varphi' \in \mathfrak{h} : \|\varphi\| = \|\varphi'\| = 1} |\langle \varphi, C\varphi' \rangle|.$$

Proof: Assume the hypothesis of the lemma, one has

$$\|C\|_{\mathcal{B}(\mathfrak{h})} = \sup_{\varphi' \in \mathfrak{h} : \|\varphi'\| = 1} \|C\varphi'\|_{\mathfrak{h}}.$$

Taking $C\varphi' \neq 0$, otherwise there is nothing to prove, it is sufficient to show that:

$$\|C\varphi'\|_{\mathfrak{h}} = \sup_{\varphi\in\mathfrak{h}:\|\varphi\|=1} |\langle \varphi, C\varphi' \rangle|.$$

By Cauchy-Schwarz inequality, one has

$$\|C\varphi'\|_{\mathfrak{h}} \geq \sup_{\varphi\in\mathfrak{h}:\|\varphi\|=1} |\langle \varphi, C\varphi' \rangle|.$$

Let us take $\varphi = \frac{C\varphi'}{\|C\varphi'\|_{\mathfrak{h}}}$, where $\|\varphi\|_{\mathfrak{h}} = 1$, then

$$|\langle \varphi, C\varphi' \rangle| = \|C\varphi'\|_{\mathfrak{h}}$$

and so

$$\|C\varphi'\|_{\mathfrak{h}} \leq \sup_{\varphi\in\mathfrak{h}:\|\varphi\|=1} |\langle \varphi, C\varphi' \rangle|.$$

■

Lemma 7.2.2 (Operator norm estimate-II)
For any operator $C \in \mathcal{B}(\mathfrak{h})$,

$$\|C\|_{\mathcal{B}(\mathfrak{h})} \leq \sup_{x\in\mathbb{Z}^d} \sum_{y\in\mathbb{Z}^d} \left| \left\langle \mathrm{e}_x, C\mathrm{e}_y \right\rangle_{\mathfrak{h}} \right|.$$

Proof: By the Cauchy-Schwarz inequality, for all $\varphi, \psi \in \mathfrak{h}$,

$$\begin{aligned}
\left|\langle \varphi, C\psi \rangle_{\mathfrak{h}}\right| &\leq \sum_{x,y\in\mathbb{Z}^d} \left| \varphi(x)\psi(y) \left\langle \mathrm{e}_x, C\mathrm{e}_y \right\rangle_{\mathfrak{h}} \right| \\
&= \sum_{x,y\in\mathbb{Z}^d} \left(|\varphi(x)| \left| \left\langle \mathrm{e}_x, C\mathrm{e}_y \right\rangle_{\mathfrak{h}} \right|^{1/2} \right) \left(|\psi(y)| \left| \left\langle \mathrm{e}_x, C\mathrm{e}_y \right\rangle_{\mathfrak{h}} \right|^{1/2} \right) \\
&\leq \sqrt{\sum_{x,y\in\mathbb{Z}^d} \left(|\varphi(x)|^2 \left| \left\langle \mathrm{e}_x, C\mathrm{e}_y \right\rangle_{\mathfrak{h}} \right| \right)} \sqrt{\sum_{x,y\in\mathbb{Z}^d} |\psi(y)|^2 \left| \left\langle \mathrm{e}_x, C\mathrm{e}_y \right\rangle_{\mathfrak{h}} \right|} \\
&\leq \|\varphi\|_{\mathfrak{h}} \|\psi\|_{\mathfrak{h}} \sup_{x\in\mathbb{Z}^d} \sum_{y\in\mathbb{Z}^d} \left| \left\langle \mathrm{e}_x, C\mathrm{e}_y \right\rangle_{\mathfrak{h}} \right|.
\end{aligned}$$

We conclude by using lemma 7.2.1. ■

The last one is a version of the Bogoliubov inequality. Recall that the tracial state tr is the quasi-free state satisfying (4.20) at $\beta = 0$.

Lemma 7.2.3 (Bogoliubov-type inequalities)
Let $C \in \mathcal{U}$ be any strictly positive element.
(i) *For any continuously differentiable family $\{H_\alpha\}_{\alpha\in\mathbb{R}} \subset \mathcal{U}$ of self-adjoint elements,*

$$\left|\partial_\alpha \ln \mathrm{tr}\left(C\mathrm{e}^{H_\alpha}\right)\right| \leq \sup_{u\in[-1/2,1/2]} \left\|\mathrm{e}^{uH_\alpha}\left\{\partial_\alpha H_\alpha\right\}\mathrm{e}^{-uH_\alpha}\right\|_{\mathcal{U}} .$$

(ii) *Similarly, for any self-adjoint $H_0, H_1 \in \mathcal{U}$,*

$$\left|\ln \mathrm{tr}\left(C\mathrm{e}^{H_1}\right) - \ln \mathrm{tr}\left(C\mathrm{e}^{H_0}\right)\right| \leq \sup_{\alpha\in[0,1]} \sup_{u\in[-1/2,1/2]} \left\|\mathrm{e}^{u(\alpha H_1+(1-\alpha)H_0)}\left(H_1 - H_0\right)\mathrm{e}^{-u(\alpha H_1+(1-\alpha)H_0)}\right\|_{\mathcal{U}} .$$

Proof: (i) By Duhamel's formula, for any continuously differentiable family $\{H_\alpha\}_{\alpha\in\mathbb{R}} \subset \mathcal{U}$ of self-adjoint elements,

$$\partial_\alpha\left\{\mathrm{e}^{H_\alpha}\right\} = \int_0^1 \mathrm{e}^{uH_\alpha}\left\{\partial_\alpha H_\alpha\right\}\mathrm{e}^{(1-u)H_\alpha}\mathrm{d}u,$$

which implies that

$$\partial_\alpha \ln \mathrm{tr}\left(C\mathrm{e}^{H_\alpha}\right) = \int_0^1 \frac{\mathrm{tr}\left(C\mathrm{e}^{uH_\alpha}\left\{\partial_\alpha H_\alpha\right\}\mathrm{e}^{(1-u)H_\alpha}\right)}{\mathrm{tr}\left(C\mathrm{e}^{H_\alpha}\right)}\mathrm{d}u.$$

Using the cyclicity of the trace, we then get

$$\begin{aligned}\partial_\alpha \ln \mathrm{tr}\left(C\mathrm{e}^{H_\alpha}\right) &= \int_0^1 \frac{\mathrm{tr}\left(\mathrm{e}^{\frac{H_\alpha}{2}}C\mathrm{e}^{\frac{H_\alpha}{2}}\mathrm{e}^{\left(u-\frac{1}{2}\right)H_\alpha}\left\{\partial_\alpha H_\alpha\right\}\mathrm{e}^{\left(\frac{1}{2}-u\right)H_\alpha}\right)}{\mathrm{tr}\left(\mathrm{e}^{\frac{H_\alpha}{2}}C\mathrm{e}^{\frac{H_\alpha}{2}}\right)}\mathrm{d}u \\ &= \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{\mathrm{tr}\left(\mathrm{e}^{\frac{H_\alpha}{2}}C\mathrm{e}^{\frac{H_\alpha}{2}}\mathrm{e}^{uH_\alpha}\left\{\partial_\alpha H_\alpha\right\}\mathrm{e}^{-uH_\alpha}\right)}{\mathrm{tr}\left(\mathrm{e}^{\frac{H_\alpha}{2}}C\mathrm{e}^{\frac{H_\alpha}{2}}\right)}\mathrm{d}u,\end{aligned}$$

which yields (i).
(ii) To prove the second assertion, it suffices to apply Assertion (i) to the family defined by

$$H_\alpha = H_0 + \alpha\left(H_1 - H_0\right), \qquad \alpha \in [0,1] .$$

∎

Observe that Lemma 7.2.3 (ii) is proven in [48, Lemma 3.6]. Here, we give a proof of this estimate for completeness. These Bogoliubov-type inequalities are useful because we deal with quasi-free dynamics. In this case, we have a very good control on the norm of

$$\mathrm{e}^{uH_\alpha}\left\{\partial_\alpha H_\alpha\right\}\mathrm{e}^{-uH_\alpha},$$

because H_α is a bilinear element, as we will see in the sequel. As explained in Section 3.2.3, bilinear elements can be used to represent the dynamics $\{\tau_t^{(\omega,\mathcal{Z})}\}_{t\in\mathbb{R}}$ for any $\omega \in \Omega$

and $\mathcal{Z} \in \mathfrak{Z}_{\mathrm{f}}$. See (4.18), replacing $h^{(\omega)}$ with $h^{(\omega)}_{\mathcal{Z}}$ (cf. (4.10)), and observe that the range of $h^{(\omega)}_{\mathcal{Z}} \in \mathcal{B}(\mathfrak{h})$ is finite dimensional whenever $\mathcal{Z} \in \mathfrak{Z}_{\mathrm{f}}$. Additionally, by using the tracial state tr, i.e., the quasi-free state satisfying (4.20) for $\beta = 0$, the corresponding KMS state defined by (4.20) by replacing $h^{(\omega)}$ in this equation with $h^{(\omega)}_{\mathcal{Z}}$ (see (4.10)) is explicity given by

$$\varrho^{(\omega)}_{\mathcal{Z}}(B) = \frac{\mathrm{tr}\left(B\mathrm{e}^{-\beta\langle \mathrm{A}, h^{(\omega)}_{\mathcal{Z}} \mathrm{A}\rangle}\right)}{\mathrm{tr}\left(\mathrm{e}^{-\beta\langle \mathrm{A}, h^{(\omega)}_{\mathcal{Z}} \mathrm{A}\rangle}\right)}, \qquad B \in \mathcal{U}, \tag{7.1}$$

for any $\omega \in \Omega$, $\lambda, \vartheta \in \mathbb{R}^+_0$, $\beta \in \mathbb{R}^+$ and $\mathcal{Z} \in \mathfrak{Z}_{\mathrm{f}}$. We conclude now by an additional observation used later to control quantum fluctuations:

Lemma 7.2.4
For any self-adjoint operators $C_1, C_2 \in \mathcal{B}(\mathfrak{h})$ whose ranges are finite dimensional, let $C := \ln\left(\mathrm{e}^{C_2}\mathrm{e}^{C_1}\mathrm{e}^{C_2}\right)$. Then,

$$\mathrm{ran}(C) \subset \mathrm{lin}\,\{\mathrm{ran}(C_1) \cup \mathrm{ran}(C_2)\}$$

and there is a constant $D \in \mathbb{R}$ such that

$$\mathrm{e}^{\langle \mathrm{A}, C_2 \mathrm{A}\rangle}\mathrm{e}^{\langle \mathrm{A}, C_1 \mathrm{A}\rangle}\mathrm{e}^{\langle \mathrm{A}, C_2 \mathrm{A}\rangle} = \mathrm{e}^{\langle \mathrm{A}, C \mathrm{A}\rangle + D\mathbf{1}_{\mathcal{U}}}.$$

Proof: Fix all parameters of the lemma. We give the proof in two steps:

Step 1: Let

$$\mathfrak{h}_0 := \mathrm{lin}\,\{\mathrm{ran}(C_1) \cup \mathrm{ran}(C_2)\}$$

and $\mathcal{U}_{\mathfrak{h}_0} \subset \mathcal{U} \equiv \mathcal{U}_{\mathfrak{h}}$ be the (finite dimensional) CAR C^*–subalgebra generated by the identity $\mathbf{1}_{\mathcal{U}}$ and $\{a(\varphi)\}_{\varphi \in \mathfrak{h}_0}$. Take two strictly positive elements M_1, M_2 of $\mathcal{U}_{\mathfrak{h}_0}$ satisfying the conditions

$$M_1 a(\varphi) M_1^{-1} = M_2 a(\varphi) M_2^{-1} \qquad \text{and} \qquad M_1 a(\varphi)^* M_1^{-1} = M_2 a(\varphi)^* M_2^{-1}$$

for any $\varphi \in \mathfrak{h}_0$. From this we conclude that

$$M_1 A M_1^{-1} = M_2 A M_2^{-1}, \qquad A \in \mathcal{U}_{\mathfrak{h}_0},$$

because all elements of $\mathcal{U}_{\mathfrak{h}_0}$ are polynomials in $\{a(\varphi), a(\varphi)^*\}_{\varphi \in \mathfrak{h}_0}$, by definition of $\mathcal{U}_{\mathfrak{h}_0}$ and finite dimensionality of $\mathfrak{h}_0$. In particular, by choosing, respectively, $A = M_2^{-1}$ and $A = M_2^{-1} B M_2$ for $B \in \mathcal{U}_{\mathfrak{h}_0}$, it follows that

$$M_1 M_2^{-1} = M_2^{-1} M_1 \qquad \text{and} \qquad M_1 M_2^{-1} B = B M_1 M_2^{-1}.$$

Hence, since any element of $\mathcal{U}_{\mathfrak{h}_0}$ commuting with all elements of $\mathcal{U}_{\mathfrak{h}_0}$ is a multiple of the identity, there is $D \in \mathbb{C}$ such that

$$M_1 M_2^{-1} = M_2^{-1} M_1 = D\mathbf{1}_{\mathcal{U}}.$$

The constant D is non-zero because M_1, M_2 are assumed to be invertible. In fact, $M_1 = DM_2$ with $D > 0$ because $M_1, M_2 > 0$.

Step 2: Observe that $\mathrm{e}^{C_2}\mathrm{e}^{C_1}\mathrm{e}^{C_2} > 0$ because C_1, C_2 are both self-adjoint operators. In particular, $C := \ln\left(\mathrm{e}^{C_2}\mathrm{e}^{C_1}\mathrm{e}^{C_2}\right)$ is well-defined as a bounded self-adjoint operator acting on $\mathfrak{h}$ with $\mathrm{ran}(C) \subset \mathfrak{h}_0$. Using (3.19), we obtain that

$$\mathrm{e}^{\langle \mathrm{A},C\mathrm{A}\rangle} a(\varphi) \mathrm{e}^{-\langle \mathrm{A},C\mathrm{A}\rangle} = \mathrm{e}^{\langle \mathrm{A},C_2\mathrm{A}\rangle}\mathrm{e}^{\langle \mathrm{A},C_1\mathrm{A}\rangle}\mathrm{e}^{\langle \mathrm{A},C_2\mathrm{A}\rangle} a(\varphi) \mathrm{e}^{-\langle \mathrm{A},C_2\mathrm{A}\rangle}\mathrm{e}^{-\langle \mathrm{A},C_1\mathrm{A}\rangle}\mathrm{e}^{-\langle \mathrm{A},C_2\mathrm{A}\rangle}$$

and

$$\mathrm{e}^{\langle \mathrm{A},C\mathrm{A}\rangle} a(\varphi)^* \mathrm{e}^{-\langle \mathrm{A},C\mathrm{A}\rangle} = \mathrm{e}^{\langle \mathrm{A},C_2\mathrm{A}\rangle}\mathrm{e}^{\langle \mathrm{A},C_1\mathrm{A}\rangle}\mathrm{e}^{\langle \mathrm{A},C_2\mathrm{A}\rangle} a(\varphi)^* \mathrm{e}^{-\langle \mathrm{A},C_2\mathrm{A}\rangle}\mathrm{e}^{-\langle \mathrm{A},C_1\mathrm{A}\rangle}\mathrm{e}^{-\langle \mathrm{A},C_2\mathrm{A}\rangle}.$$

By Step 1, the assertion follows. ■

Note that another proof of the same result is given by J.L. Lebowitz, M. Lenci and H. Spohn in 2005, see [47, Lemma IV.1].

7.3 Bilinear elements associated with currents

For simplicity, below we fix $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$, and $\eta, \mu \in \mathbb{R}^+$ once and for all. For any $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$, any collection $\mathcal{Z}^{(\tau)} \in \mathfrak{Z}$, $\mathcal{Z} \in \mathfrak{Z}_{\mathrm{f}}$, and $\lambda, \vartheta \in \mathbb{R}_0^+$, $\omega \in \Omega$, we define the observables

$$\mathfrak{K}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} := \sum_{k,q=1}^{d} w_k \sum_{Z\in\mathcal{Z}} \sum_{x,y,x+e_k,y+e_q\in Z} \int_{-\infty}^{0} \{\mathcal{E}(\alpha)\}_q \,\mathrm{d}\alpha \int_0^{-\alpha} \mathrm{d}s\, i[\tau_{-s}^{(\omega,\mathcal{Z}^{(\tau)})}(I_{(y+e_q,y)}^{(\omega)}), I_{(x+e_k,x)}^{(\omega)}] \tag{7.2}$$

$$+ 2\sum_{k=1}^{d} w_k \sum_{Z\in\mathcal{Z}} \sum_{x,x+e_k\in Z} \left(\int_{-\infty}^{0} \{\mathcal{E}(\alpha)\}_q \,\mathrm{d}\alpha\right) \mathfrak{Re}\left(\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle a(\mathfrak{e}_{x+e_k})^* a(\mathfrak{e}_x)\right). \tag{7.3}$$

(7.4)

Note that

$$\mathfrak{K}_{\{\Lambda\},\{\mathbb{Z}^d\}}^{(\omega,\mathcal{E})} = |\Lambda|\, \mathbb{I}_{\Lambda}^{(\omega,\mathcal{E})}, \qquad \Lambda \in \mathcal{P}_{\mathrm{f}}(\mathbb{Z}^d),$$

is a current *observable*, see Equation (4.35) and (4.33). These observables are bilinear elements as it is given Definition 3.2.2:

(i) Single-hopping operators: For any $x \in \mathbb{Z}^d$, the shift operator $s_x \in \mathcal{B}(\mathfrak{h})$ is defined by

$$(s_x\psi)(y) := \psi(x+y), \qquad y \in \mathbb{Z}^d, \tag{7.5}$$

Note that $s_x^* = s_{-x} = s_x^{-1}$ for any $x \in \mathbb{Z}^d$. Then, for any $\omega \in \Omega$ and $\vartheta \in \mathbb{R}_0^+$, the single-hopping operators are

$$S_{x,y}^{(\omega)} := \langle \mathfrak{e}_y, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}} P_{\{y\}} s_{y-x} P_{\{x\}}, \qquad x, y \in \mathbb{Z}^d, \tag{7.6}$$

where $P_{\{x\}}$ is the orthogonal projection defined by (4.9) for $\Lambda = \{x\}$. Observe that

$$\left\langle \mathrm{A}, S_{x,y}^{(\omega)} \mathrm{A} \right\rangle = \langle \mathfrak{e}_y, \Delta_{\omega,\vartheta} \mathfrak{e}_x \rangle_{\mathfrak{h}} a(\mathfrak{e}_y)^* a(\mathfrak{e}_x), \qquad x, y \in \mathbb{Z}^d.$$

Similarly, the paramagnetic current observables defined by (4.28) equal

$$I_{(x,y)}^{(\omega)} = 2\langle \mathrm{A}, \mathfrak{Im}\{S_{x,y}^{(\omega)}\} \mathrm{A} \rangle, \qquad x, y \in \mathbb{Z}^d,$$

for any $\omega \in \Omega$ and $\vartheta \in \mathbb{R}_0^+$. See equation (3.16).

(ii) Local current observables: By (3.18), for any $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, any collection $\mathcal{Z}^{(\tau)} \in \mathfrak{Z}$, $\mathcal{Z} \in \mathfrak{Z}_{\mathrm{f}}$, and $\lambda, \vartheta \in \mathbb{R}_0^+$, $\omega \in \Omega$,

$$\mathfrak{K}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} = \left\langle \mathrm{A}, K_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} \mathrm{A} \right\rangle, \tag{7.7}$$

where

$$K_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} := 4 \sum_{k,q=1}^{d} w_k \sum_{Z \in \mathcal{Z}} \sum_{x,y,x+e_k,y+e_q \in Z} \int_{-\infty}^{0} \{\mathcal{E}(\alpha)\}_q \, \mathrm{d}\alpha \tag{7.8}$$

$$\int_0^{-\alpha} \mathrm{d}s \; i \left[\mathrm{e}^{-ish_{\mathcal{Z}^{(\tau)}}^{(\omega)}} \mathfrak{Im}\{S_{y+e_q,y}^{(\omega)}\} \mathrm{e}^{ish_{\mathcal{Z}^{(\tau)}}^{(\omega)}}, \mathfrak{Im}\{S_{x+e_k,x}^{(\omega)}\} \right] \tag{7.9}$$

$$+ 2 \sum_{k=1}^{d} w_k \sum_{Z \in \mathcal{Z}} \sum_{x,x+e_k \in Z} \left(\int_{-\infty}^{0} \{\mathcal{E}(\alpha)\}_k \, \mathrm{d}\alpha \right) \mathfrak{Re}\{S_{x+e_k,x}^{(\omega)}\} \tag{7.10}$$

is an operator acting on $\mathfrak{h}$ whose range is finite dimensional. This one-particle operator satisfies the following decay bounds:

Lemma 7.3.1 (Decay of local currents)
For any $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, $\lambda, \vartheta \in \mathbb{R}_0^+$, $\omega \in \Omega$, $x, y \in \mathbb{Z}^d$, and two collections $\mathcal{Z} \in \mathfrak{Z}_f$ and $\mathcal{Z}^{(\tau)} \in \mathfrak{Z}_f$,

$$\left| \left\langle \mathfrak{e}_x, K_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} \mathfrak{e}_y \right\rangle_{\mathfrak{h}} \right| \leq D_{7.3.1} \left(\int_{\mathbb{R}} \|\mathcal{E}(\alpha)\|_{\mathbb{R}^d} \, \mathrm{e}^{2|\alpha\eta|} \mathrm{d}\alpha \right) \left(\mathrm{e}^{-\mu_\eta |x-y|} + \eta \delta_{1,|x-y|} \right),$$

$$\frac{1}{|\cup \mathcal{Z}|} \sum_{x,y \in \mathbb{Z}^d} \left| \left\langle \mathfrak{e}_x, K_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} \mathfrak{e}_y \right\rangle_{\mathfrak{h}} \right| \leq D_{7.3.1} \left(\int_{\mathbb{R}} \|\mathcal{E}(\alpha)\|_{\mathbb{R}^d} \, \mathrm{e}^{2|\alpha\eta|} \mathrm{d}\alpha \right) \sum_{z \in \mathbb{Z}^d} \mathrm{e}^{-\mu_\eta |z|} (1 + \eta),$$

where

$$D_{7.3.1} := 4d\eta^{-1} \times 36^2 (1 + \vartheta)^2 \sum_{z \in \mathbb{Z}^d} \mathrm{e}^{2\mu_\eta (1-|z|)} < \infty.$$

Recall that μ_η is defined by (4.14).

Proof: Fix the parameters of the lemma. By (4.13), note that for any $z_1, z_2, x, y \in \mathbb{Z}^d$, $\omega \in \Omega$, $\vartheta \in \mathbb{R}_0^+$ and $s \in \mathbb{R}$,

$$\left|\left\langle \mathfrak{e}_x, \mathrm{e}^{-ish^{(\omega)}_{\mathcal{Z}^{(\tau)}}} S^{(\omega)}_{z_2+e_q,z_2} \mathrm{e}^{ish^{(\omega)}_{\mathcal{Z}^{(\tau)}}} S^{(\omega)}_{z_1+e_k,z_1} \mathfrak{e}_y \right\rangle_{\mathfrak{h}}\right| \leq 36^2 (1+\vartheta)^2 \mathrm{e}^{2|s\eta|-2\mu_\eta\left(|x-z_2-e_q|+|y-z_2+e_k|\right)} \delta_{y,z_1}. \quad (7.11)$$

By the Cauchy-Schwarz inequality, observe also that

$$\sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-2\mu_\eta\left(|x-z|+|y-z|\right)} \leq \mathrm{e}^{-\mu_\eta|x-y|} \sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-\mu_\eta\left(|x-z|+|y-z|\right)} \leq \mathrm{e}^{-\mu_\eta|x-y|} \left(\sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-2\mu_\eta|z|}\right). \quad (7.12)$$

From (7.11)-(7.12), we obtain the bound

$$\sum_{Z\in\mathcal{Z}} \sum_{z_1,z_2,z_1+e_k,z_2+e_q\in Z} \left|\left\langle \mathfrak{e}_x, \mathrm{e}^{-ish^{(\omega)}_{\mathcal{Z}^{(\tau)}}} S^{(\omega)}_{z_2+e_q,z_2} \mathrm{e}^{ish^{(\omega)}_{\mathcal{Z}^{(\tau)}}} S^{(\omega)}_{z_1+e_k,z_1} \mathfrak{e}_y \right\rangle_{\mathfrak{h}}\right| \quad (7.13)$$

$$\leq 36^2 (1+\vartheta)^2 \mathrm{e}^{2|s\eta|-\mu_\eta|x-y|} \left(\sum_{z\in\mathbb{Z}^d} \mathrm{e}^{2\mu_\eta(1-|z|)}\right), \quad (7.14)$$

using that $|z - e_k| \geq |z| - 1$ for any $z \in \mathbb{Z}^d$ and $k \in \{1, \ldots, d\}$. The other terms computed from (7.10) are estimated in the same way. We omit the details. This yields the first bound of the lemma. The second estimate is also proven in the same way. ■

Corollary 7.3.2
For any $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, $\lambda, \vartheta \in \mathbb{R}_0^+$, $\omega \in \Omega$, $x, y \in \mathbb{Z}^d$, and two collections $\mathcal{Z} \in \mathfrak{Z}_f$ and $\mathcal{Z}^{(\tau)} \in \mathfrak{Z}_f$,

$$\sup_{x\in\mathbb{Z}^d} \sum_{y\in\mathbb{Z}^d} \left|\left\langle \mathfrak{e}_x, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \mathfrak{e}_y \right\rangle_{\mathfrak{h}}\right| \leq D_{7.3.1} \left(\int_{\mathbb{R}} \|\mathcal{E}(\alpha)\|_{\mathbb{R}^d} \mathrm{e}^{2|\alpha\eta|} \mathrm{d}\alpha\right) \left(\sum_{y\in\mathbb{Z}^d} \mathrm{e}^{-\mu_\eta|y|} + 2d\eta\right).$$

Proof: This is a direct consequence of Lemma 7.3.1. ■

It is convenient to introduce at this point the notation

$$\partial_\Lambda(\tilde{\Lambda}) := \left\{\{x, y\} \subset \Lambda \colon \left|x - y\right| = 1,\ \{x, y\} \cap \tilde{\Lambda} \neq \emptyset \text{ and } \{x, y\} \cap \tilde{\Lambda}^c \neq \emptyset\right\} \quad (7.15)$$

for any set $\tilde{\Lambda} \subset \Lambda \subset \mathbb{Z}^d$ with complement $\tilde{\Lambda}^c := \mathbb{Z}^d \backslash \tilde{\Lambda}$, while, for any $\mathcal{Z} \in \mathfrak{Z}$,

$$\partial_\Lambda(\mathcal{Z}) := \{\partial_\Lambda(Z) : Z \in \mathcal{Z}\}.$$

Then, the one-particle operators (7.10) also satisfy the following bounds:

Lemma 7.3.3 (Box decomposition of local currents - I)
For any $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$, $\Lambda, \tilde{\Lambda} \in \mathcal{P}_f(\mathbb{Z}^d)$, $\lambda, \vartheta \in \mathbb{R}_0^+$, $\omega \in \Omega$, *and* $\mathcal{Z} \in \mathfrak{Z}_f$ *with* $\cup\mathcal{Z} \subset \tilde{\Lambda}$,

$$\sum_{x,y\in\mathbb{Z}^d} \left| \left\langle \mathrm{e}_x, \left(K^{(\omega,\mathcal{E})}_{\{\Lambda\},\{\tilde{\Lambda}\}} - K^{(\omega,\mathcal{E})}_{\{\Lambda\},\mathcal{Z}} \right) \mathrm{e}_y \right\rangle_{\mathfrak{h}} \right|$$
$$\leq D_{7.3.3} \left(\int_{\mathbb{R}} \|\mathcal{E}(\alpha)\|_{\mathbb{R}^d} \alpha^2 \mathrm{e}^{2|\alpha\eta|} \mathrm{d}\alpha \right) \left(\sum_{x\in\Lambda} \sum_{z\in\tilde{\Lambda}\setminus\cup\mathcal{Z}} \mathrm{e}^{-\mu_\eta|x-z|} + \sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-\mu_\eta|z|} \sum_{x\in\cup\partial_{\tilde{\Lambda}}(\mathcal{Z})} 1 \right),$$

where

$$D_{7.3.3} := 8\times 36^4 (1+\vartheta)^3 (4d+\lambda)\, \mathrm{e}^{3\mu_\eta} \left(\sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-\mu_\eta|z|} \right)^3 < \infty.$$

Proof: Fix all parameters of the lemma. Let

$$C^{(\omega)}_{\mathcal{Z}}(z_1,z_2,k,q) = \int_0^{-\alpha} \mathrm{d}s\, i \left[\mathrm{e}^{-ish^{(\omega)}_{\mathcal{Z}}} \mathfrak{Im}\{S^{(\omega)}_{z_2+e_q,z_2}\} \mathrm{e}^{ish^{(\omega)}_{\mathcal{Z}}}, \mathfrak{Im}\{S^{(\omega)}_{z_1+e_k,z_1}\} \right]$$

for any $z_1, z_2 \in \mathbb{Z}^d$ and $k, q \in \{1,\ldots,d\}$. By Duhamel's formula,

$$\begin{aligned} &\mathrm{e}^{-ish^{(\omega)}_{\{\tilde{\Lambda}\}}} A \mathrm{e}^{ish^{(\omega)}_{\{\tilde{\Lambda}\}}} - \mathrm{e}^{-ish^{(\omega)}_{\mathcal{Z}}} A \mathrm{e}^{ish^{(\omega)}_{\mathcal{Z}}} \\ &= -i \int_0^s \mathrm{e}^{-i(s-u)h^{(\omega)}_{\mathcal{Z}}} \left[h^{(\omega)}_{\{\tilde{\Lambda}\}} - h^{(\omega)}_{\mathcal{Z}}, \mathrm{e}^{-iuh^{(\omega)}_{\{\tilde{\Lambda}\}}} A \mathrm{e}^{iuh^{(\omega)}_{\{\tilde{\Lambda}\}}} \right] \mathrm{e}^{i(s-u)h^{(\omega)}_{\mathcal{Z}}} \mathrm{d}u \end{aligned}$$

and hence, for any $z_1, z_2 \in \mathbb{Z}^d$ and $k, q \in \{1,\ldots,d\}$,

$$\begin{aligned} C^{(\omega)}_{\{\tilde{\Lambda}\}}(z_1,z_2,k,q) - C^{(\omega)}_{\mathcal{Z}}(z_1,z_2,k,q) &= 4 \int_0^{\alpha} \mathrm{d}s \int_0^s \mathrm{d}u \\ &\left[\mathrm{e}^{-i(s-u)h^{(\omega)}_{\mathcal{Z}}} \left[h^{(\omega)}_{\{\tilde{\Lambda}\}} - h^{(\omega)}_{\mathcal{Z}}, \mathrm{e}^{-iuh^{(\omega)}_{\{\tilde{\Lambda}\}}} \mathfrak{Im}\{S^{(\omega)}_{z_2+e_q,z_2}\} \mathrm{e}^{iuh^{(\omega)}_{\{\tilde{\Lambda}\}}} \right] \mathrm{e}^{i(s-u)h^{(\omega)}_{\mathcal{Z}}}, \mathfrak{Im}\{S^{(\omega)}_{z_1+e_k,z_1}\} \right]. \end{aligned}$$

By developing the commutators and $\mathfrak{Im}\{\cdot\}$ we get sixteen terms:

$$C^{(\omega)}_{\{\tilde{\Lambda}\}}(z_1,z_2,k,q) - C^{(\omega)}_{\mathcal{Z}}(z_1,z_2,k,q) = \int_0^{\alpha} \mathrm{d}s \int_0^s \mathrm{d}u \sum_{j=1}^{16} \mathbf{X}_j(s,u,z_1,z_2), \tag{7.16}$$

where, for instance,

$$\mathbf{X}_1(s,u,z_1,z_2) := \mathrm{e}^{-i(s-u)h^{(\omega)}_{\mathcal{Z}}} \left(h^{(\omega)}_{\{\tilde{\Lambda}\}} - h^{(\omega)}_{\mathcal{Z}} \right) \mathrm{e}^{-iuh^{(\omega)}_{\{\tilde{\Lambda}\}}} S_{z_2+e_q,z_2} \mathrm{e}^{iuh^{(\omega)}_{\{\tilde{\Lambda}\}}} \mathrm{e}^{i(s-u)h^{(\omega)}_{\mathcal{Z}}} S_{z_1+e_k,z_1}. \tag{7.17}$$

Since $\cup\mathcal{Z} \subset \tilde{\Lambda}$, note that

$$h^{(\omega)}_{\{\tilde{\Lambda}\}} - h^{(\omega)}_{\mathcal{Z}} = \sum_{z_3,z_4\in\tilde{\Lambda}\setminus\cup\mathcal{Z}\,:\,|z_3-z_4|=1} S^{(\omega)}_{z_3,z_4} + \sum_{Z\in\mathcal{Z}} \sum_{\{z_3,z_4\}\in\partial_{\tilde{\Lambda}}(Z)} \left(S^{(\omega)}_{z_3,z_4} + S^{(\omega)}_{z_4,z_3} \right) \tag{7.18}$$
$$+ \sum_{z_3\in\tilde{\Lambda}\setminus\cup\mathcal{Z}} \lambda\omega_1(z_3)\, S^{(\omega)}_{z_3,z_3}. \tag{7.19}$$

Meanwhile, for any $z_1, z_2, z_3, z_4, x, y \in \mathbb{Z}^d$ with $|z_3 - z_4| \leq 1$, and real numbers $s \geq u \geq 0$, we infer from (4.13) and (7.12) that

$$\left| \left\langle \mathfrak{e}_x, \mathrm{e}^{-i(s-u)h^{(\omega)}_{\mathcal{Z}}} S_{z_3,z_4} \mathrm{e}^{-iuh^{(\omega)}_{\{\tilde{\Lambda}\}}} S^{(\omega)}_{z_2+e_q,z_2} \mathrm{e}^{iuh^{(\omega)}_{\{\tilde{\Lambda}\}}} \mathrm{e}^{i(s-u)h^{(\omega)}_{\mathcal{Z}}} S^{(\omega)}_{z_1+e_k,z_1} \mathfrak{e}_y \right\rangle_{\mathfrak{h}} \right| \\ \leq 36^4 (1+\vartheta)^3 \mathrm{e}^{2|s\eta|+3\mu_\eta} \left(\sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-2\mu_\eta |z|} \right) \delta_{z_1,y} \mathrm{e}^{-\mu_\eta \left(|z_2-y|+|x-z_3|+|z_3-z_2| \right)}.$$

By (7.17)-(7.19), for any $\alpha \geq 0$, it follows that

$$\sum_{x,y\in\mathbb{Z}^d} \sum_{z_1,z_2,z_1+e_k,z_2+e_q\in\Lambda} \int_0^\alpha \mathrm{d}s \int_0^s \mathrm{d}u \left| \left\langle \mathfrak{e}_x, \mathbf{X}_1 (s,u,z_1,z_2) \mathfrak{e}_y \right\rangle_{\mathfrak{h}} \right| \\ \leq \frac{36^4}{2} (1+\vartheta)^3 (4d+\lambda) \alpha^2 \mathrm{e}^{2|\alpha\eta|+3\mu_\eta} \left(\sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-\mu_\eta |z|} \right)^3 \\ \times \left(\sum_{x\in\Lambda} \sum_{z\in\tilde{\Lambda}\setminus\cup\mathcal{Z}} \mathrm{e}^{-\mu_\eta |x-z|} + \sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-\mu_\eta |z|} \sum_{x\in\cup\partial_{\tilde{\Lambda}}(\mathcal{Z})} 1 \right).$$

The fifteen other terms $\mathbf{X}_j$ in (7.16) satisfy the same bound. By (7.10), the assertion follows for any $\mathcal{E} \in C_0^\infty(\mathbb{R};\mathbb{R}^d)$. ■

Lemma 7.3.4 (Box decomposition of local currents - II)
For any $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$, $\Lambda \in \mathcal{P}_f(\mathbb{Z}^d)$, $\lambda, \vartheta \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\mathcal{Z}_\tau \in \mathfrak{Z}$, *and* $\mathcal{Z} \in \mathfrak{Z}_f$ *with* $\cup\mathcal{Z} \subset \Lambda$,

$$\sum_{x,y\in\mathbb{Z}^d} \left| \left\langle \mathfrak{e}_x, \left(K^{(\omega,\mathcal{E})}_{\{\Lambda\},\mathcal{Z}_\tau} - K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}_\tau} \right) \mathfrak{e}_y \right\rangle_{\mathfrak{h}} \right| \leq D_{7.3.4} \left(\int_{\mathbb{R}} \|\mathcal{E}(\alpha)\|^2_{\mathbb{R}^d} |\alpha| \mathrm{e}^{2|\alpha\eta|} \mathrm{d}\alpha \right) \sum_{z\in(\Lambda\setminus\cup\mathcal{Z})\cup(\cup\partial_\Lambda(\mathcal{Z}))} 1,$$

where

$$D_{7.3.4} := 16 \times 36^2 (1+\vartheta)^2 d\mathrm{e}^{4\mu_\eta} \left(\sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-2\mu_\eta |z|} \right)^2 + d(1+\vartheta) < \infty.$$

Proof: Fix all parameters of the lemma. By combining (7.11) with direct estimates we observe that

$$\sum_{x,y\in\mathbb{Z}^d} \sum_{z_1,z_2,z_1+e_k,z_2+e_q\in\Lambda} \left| \left\langle \mathfrak{e}_x, \mathrm{e}^{-ish^{(\omega)}_{\mathcal{Z}^{(\tau)}}} S^{(\omega)}_{z_2+e_q,z_2} \mathrm{e}^{ish^{(\omega)}_{\mathcal{Z}^{(\tau)}}} S^{(\omega)}_{z_1+e_k,z_1} \mathfrak{e}_y \right\rangle_{\mathfrak{h}} \right| \tag{7.20}$$

$$- \sum_{x,y\in\mathbb{Z}^d} \sum_{Z\in\mathcal{Z}} \sum_{z_1,z_2,z_1+e_k,z_2+e_q\in Z} \left| \left\langle \mathfrak{e}_x, \mathrm{e}^{-ish^{(\omega)}_{\mathcal{Z}^{(\tau)}}} S^{(\omega)}_{z_2+e_q,z_2} \mathrm{e}^{ish^{(\omega)}_{\mathcal{Z}^{(\tau)}}} S^{(\omega)}_{z_1+e_k,z_1} \mathfrak{e}_y \right\rangle_{\mathfrak{h}} \right| \tag{7.21}$$

$$\leq 2 \times 36^2 (1+\vartheta)^2 \mathrm{e}^{2|s\eta|+4\mu_\eta} \left(\sum_{x\in\mathbb{Z}^d} \mathrm{e}^{-2\mu_\eta |x|} \right)^2 \sum_{z\in(\Lambda\setminus\cup\mathcal{Z})\cup(\cup\partial_\Lambda(\mathcal{Z}))} 1 \tag{7.22}$$

for any $s \in \mathbb{R}$. Similar to (7.16), the quantity

$$\sum_{x,y\in\mathbb{Z}^d} \left| \left\langle \mathfrak{e}_x, \left(K^{(\omega,\mathcal{E})}_{\{\Lambda\},\mathcal{Z}_\tau} - K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}_\tau} \right) \mathfrak{e}_y \right\rangle_{\mathfrak{h}} \right|$$

is a sum of nine terms. The first one is (7.22), the last one is related to $\mathfrak{Re}\{S^{(\omega)}_{x+e_k,x}\}$ and gives the constant $d(1+\vartheta)$ in $D_{7.3.4}$. The seven remaining ones satisfy the same bound as the first one. ■

7.4 Finite-volume generating functions

Fix $\beta \in \mathbb{R}^+$ and $\lambda, \vartheta \in \mathbb{R}^+_0$. Given $\mathcal{E} \in C^0_0(\mathbb{R};\mathbb{R}^d)$, $\omega \in \Omega$ and three finite collections $\mathcal{Z}, \mathcal{Z}^{(\varrho)}, \mathcal{Z}^{(\tau)} \in \mathfrak{Z}_{\mathrm{f}}$, we define the finite-volume generating function

$$\mathrm{J}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} := g^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} - g^{(\omega,0)}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}, \tag{7.23}$$

where

$$g^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} := \frac{1}{|\cup \mathcal{Z}|} \ln \mathrm{tr}\left(\mathrm{e}^{(-\beta\langle \mathrm{A}, h^{(\omega)}_{\mathcal{Z}^{(\varrho)}} \mathrm{A}\rangle)} \mathrm{e}^{(\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}})} \right). \tag{7.24}$$

Recall that the tracial state tr is the quasi-free state satisfying (4.20) at $\beta = 0$, and $h^{(\omega)}_{\mathcal{Z}^{(\varrho)}}$ is the one-particle Hamiltonian defined by (4.10). See also Definition 3.2.2 and (7.4). By construction, note that

$$\frac{1}{|\Lambda_\ell|} \ln \varrho^{(\omega)}\left(\mathrm{e}^{|\Lambda_\ell| \mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L}} \right) = \lim_{L_\varrho\to\infty} \lim_{L_\tau\to\infty} \mathrm{J}^{(\omega,\mathcal{E})}_{\{\Lambda_\ell\},\{\Lambda_{L_\varrho}\},\{\Lambda_{L_\tau}\}}. \tag{7.25}$$

The family of functions $\mathcal{E} \mapsto \mathrm{J}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}$ is equicontinuous with uniformly bounded second derivative:

Proposition 7.4.1 (Equicontinuity of generating functions)
Fix $n \in \mathbb{N}$. The family of maps $\mathcal{E} \mapsto \mathrm{J}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}$ from $C^0_0([-n,n];\mathbb{R}^d) \subset C^0_0(\mathbb{R};\mathbb{R}^d)$ to $\mathbb{R}$, for $\beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}^+_0$, $\omega \in \Omega$, $\mathcal{Z}, \mathcal{Z}^{(\varrho)}, \mathcal{Z}^{(\tau)} \in \mathfrak{Z}_f$, $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$, and ϑ in a compact set of $\mathbb{R}^+_0$, is equicontinuous with respect to the sup norm for $\mathcal{E}$ in any bounded set of $C^0_0([-n,n];\mathbb{R}^d)$.

Proof: Fix $n \in \mathbb{N}$, $\beta \in \mathbb{R}^+$, $\lambda, \vartheta \in \mathbb{R}^+_0$, $\omega \in \Omega$, $\mathcal{Z}, \mathcal{Z}^{(\varrho)}, \mathcal{Z}^{(\tau)} \in \mathfrak{Z}_{\mathrm{f}}$. By using Lemma 7.2.3 (ii), for any $\mathcal{E}_0, \mathcal{E}_1 \in C^0_0([-n,n];\mathbb{R}^d)$,

$$\left| g^{(\omega,\mathcal{E}_1)}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} - g^{(\omega,\mathcal{E}_0)}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} \right| \tag{7.26}$$

$$\leq \frac{1}{|\cup \mathcal{Z}|} \sup_{\alpha\in[0,1]} \sup_{u\in[-1/2,1/2]} \left\| \mathrm{e}^{u\mathfrak{K}^{(\omega,\alpha\mathcal{E}_1+(1-\alpha)\mathcal{E}_0)}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}} \mathfrak{K}^{(\omega,\mathcal{E}_1-\mathcal{E}_0)}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \mathrm{e}^{-u\mathfrak{K}^{(\omega,\alpha\mathcal{E}_1+(1-\alpha)\mathcal{E}_0)}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}} \right\|_{\mathcal{U}}. \tag{7.27}$$

Recall that, for any $\mathcal{E} \in C_0^\infty(\mathbb{R};\mathbb{R}^d)$, $\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}$ is the bilinear element associated with the operator $K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}$. See (7.7) and (7.10). In particular, from (3.19), we deduce the inequality

$$\sup_{u\in[-1/2,1/2]} \sup_{x,y\in\mathbb{Z}^d} \left\| \mathrm{e}^{u\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}} a(\mathfrak{e}_x)^* a\left(\mathfrak{e}_y\right) \mathrm{e}^{-u\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}} \right\|_{\mathcal{U}} \leq \mathrm{e}^{\|K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\|_{\mathcal{B}(\mathfrak{h})}}. \tag{7.28}$$

The assertion then follows by combining (7.7), (7.26) and Definition 3.2.2 with (7.28) and Lemmata 7.2.2, 7.3.1. ■

Proposition 7.4.2 (Uniform boundedness of second derivatives)
Fix $\mathcal{E} \in C_0^0\left(\mathbb{R};\mathbb{R}^d\right)$ *and* $\beta_1, s_1, \vartheta_1, \lambda_1 \in \mathbb{R}^+$. *Then,*

$$\sup_{\substack{\beta\in(0,\beta_1],\ \vartheta\in[0,\vartheta_1],\ \lambda\in[0,\lambda_1] \\ \omega\in\Omega,\ s\in[-s_1,s_1],\ \mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}\in\mathfrak{Z}_f}} \left\{ \left| \partial_s \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} \right| + \left| \partial_s^2 \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} \right| \right\} < \infty.$$

Proof: Fix the parameters of the proposition. Then, by cyclicity of the tracial state,

$$\partial_s \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} = \frac{1}{|\cup\mathcal{Z}|} \varpi_s\left(\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\right)$$

and

$$\partial_s^2 \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} = \frac{1}{|\cup\mathcal{Z}|} \left(\varpi_s\left(\left(\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\right)^2\right) - \varpi_s\left(\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\right)^2 \right), \tag{7.29}$$

where ϖ_s is the state defined, for any $B \in \mathcal{U}$, by

$$\varpi_s(B) = \frac{\mathrm{tr}\left(B \mathrm{e}^{\frac{s}{2}\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}} \mathrm{e}^{-\beta\langle \mathrm{A}, h^{(\omega)}_{\mathcal{Z}^{(\varrho)}} \mathrm{A}\rangle} \mathrm{e}^{\frac{s}{2}\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}}\right)}{\mathrm{tr}\left(\mathrm{e}^{\frac{s}{2}\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}} \mathrm{e}^{-\beta\langle \mathrm{A}, h^{(\omega)}_{\mathcal{Z}^{(\varrho)}} \mathrm{A}\rangle} \mathrm{e}^{\frac{s}{2}\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}}\right)}. \tag{7.30}$$

By Lemma 7.2.4 and (7.7), observe that ϖ_s is the quasi-free state satisfying

$$\varpi_s(a^*(\varphi)\, a(\psi)) = \left\langle \psi, \frac{1}{1+\mathrm{e}^{-\frac{s}{2}K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}} \mathrm{e}^{\beta h^{(\omega)}_{\mathcal{Z}^{(\varrho)}}} \mathrm{e}^{-\frac{s}{2}K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}}} \varphi \right\rangle_{\mathfrak{h}}, \qquad \varphi, \psi \in \mathfrak{h}. \tag{7.31}$$

Therefore, by (7.7) and Definition 3.2.2, we directly compute that

$$\partial_s \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} = \frac{1}{|\cup\mathcal{Z}|} \sum_{x,y\in\mathbb{Z}^d} \left\langle \mathfrak{e}_x, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \mathfrak{e}_y \right\rangle_{\mathfrak{h}} \varpi_s\left(a(\mathfrak{e}_x)^* a\left(\mathfrak{e}_y\right)\right)$$

and

$$\begin{aligned}\partial_s^2 \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} = \frac{1}{|\cup\mathcal{Z}|} \sum_{x,y,u,v\in\mathbb{Z}^d} & \left\langle \mathfrak{e}_x, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \mathfrak{e}_y \right\rangle_{\mathfrak{h}} \left\langle \mathfrak{e}_u, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \mathfrak{e}_v \right\rangle_{\mathfrak{h}} \\ & \times \varpi_s\left(a\left(\mathfrak{e}_y\right) a(\mathfrak{e}_u)^*\right) \varpi_s\left(a(\mathfrak{e}_x)^* a(\mathfrak{e}_v)\right),\end{aligned} \tag{7.32}$$

because of the identity

$$\omega_s\left(a(\mathfrak{e}_x)^* a(\mathfrak{e}_y) a(\mathfrak{e}_u)^* a(\mathfrak{e}_v)\right) = \omega_s\left(a(\mathfrak{e}_x)^* a(\mathfrak{e}_y)\right)\omega_s\left(a(\mathfrak{e}_u)^* a(\mathfrak{e}_v)\right) + \omega_s\left(a(\mathfrak{e}_y) a(\mathfrak{e}_u)^*\right)\omega_s\left(a(\mathfrak{e}_x)^* a(\mathfrak{e}_v)\right), \tag{7.33}$$

for $x, y, u, v \in \mathbb{Z}^d$. See Definition 3.2.10. As a consequence,

$$\left|\partial_s \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}\right| \leq \frac{1}{|\cup\mathcal{Z}|}\sum_{x,y\in\mathbb{Z}^d}\left|\left\langle \mathfrak{e}_x, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_y\right\rangle_{\mathfrak{h}}\right|$$

and

$$\left|\partial_s^2 \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}\right| \leq \sup_{u,v\in\mathbb{Z}^d}\left|\left\langle \mathfrak{e}_u, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_v\right\rangle_{\mathfrak{h}}\right|\left(\frac{1}{|\cup\mathcal{Z}|}\sum_{x,y\in\mathbb{Z}^d}\left|\left\langle \mathfrak{e}_x, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_y\right\rangle_{\mathfrak{h}}\right|\right) \tag{7.34}$$

$$\times \sup_{y\in\mathbb{Z}^d}\sum_{u\in\mathbb{Z}^d}\left|\omega_s\left(a\left(\mathfrak{e}_y\right)a\left(\mathfrak{e}_u\right)^*\right)\right|\sup_{x\in\mathbb{Z}^d}\sum_{v\in\mathbb{Z}^d}\left|\omega_s\left(a\left(\mathfrak{e}_x\right)^* a\left(\mathfrak{e}_v\right)\right)\right|, \tag{7.35}$$

which, by Lemma 7.3.1, implies that

$$\left|\partial_s \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}\right| \leq D_{7.3.1}\left(\int_{\mathbb{R}}\|\mathcal{E}(\alpha)\|_{\mathbb{R}^d}\,\mathrm{e}^{2|\alpha\eta|}\mathrm{d}\alpha\right)\sum_{z\in\mathbb{Z}^d}\mathrm{e}^{-\mu_\eta|z|}(1+\eta) \tag{7.36}$$

as well as

$$\left|\partial_s^2 \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}\right| \leq D_{7.3.1}^2\left(\int_{\mathbb{R}}\|\mathcal{E}(\alpha)\|_{\mathbb{R}^d}\,\mathrm{e}^{2|\alpha\eta|}\mathrm{d}\alpha\right)^2(1+\eta)^2\sum_{z\in\mathbb{Z}^d}\mathrm{e}^{-\mu_\eta|z|} \tag{7.37}$$

$$\times \sup_{y\in\mathbb{Z}^d}\sum_{u\in\mathbb{Z}^d}\left|\omega_s\left(a\left(\mathfrak{e}_y\right)a\left(\mathfrak{e}_u\right)^*\right)\right|\sup_{x\in\mathbb{Z}^d}\sum_{v\in\mathbb{Z}^d}\left|\omega_s\left(a\left(\mathfrak{e}_x\right)^* a\left(\mathfrak{e}_v\right)\right)\right|. \tag{7.38}$$

Again by Lemma 7.3.1 together with (4.13)-(4.14), for any $\mu > \mu_\eta$,

$$\sup_{\substack{\beta\in(0,\beta_1],\ \vartheta\in[0,\vartheta_1],\ \lambda\in[0,\lambda_1]\\ \omega\in\Omega,\ s\in[-s_1,s_1],\ \mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}\in\mathfrak{Z}_{\mathrm{f}}}}\left\{\mathbf{S}_0(sK^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}},\mu) + \mathbf{S}_0(\beta h^{(\omega)}_{\mathcal{Z}^{(\varrho)}},\mu)\right\} < \infty.$$

See (7.75). We thus infer from (7.31) and Corollary 7.7.3 that there is a constant $\mu_1 \in \mathbb{R}^+$ such that, for any $x, y \in \mathbb{Z}^d$,

$$\sup_{\substack{\beta\in(0,\beta_1],\ \vartheta\in[0,\vartheta_1],\ \lambda\in[0,\lambda_1]\\ \omega\in\Omega,\ s\in[-s_1,s_1],\ \mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}\in\mathfrak{Z}_{\mathrm{f}}}}\left|\omega_s\left(a\left(\mathfrak{e}_x\right)^* a\left(\mathfrak{e}_y\right)\right)\right| \leq 2\mathrm{e}^{-\mu_1|x-y|}. \tag{7.39}$$

Combining this estimate with (7.36)-(7.38), one gets the assertion. ■

In the next proposition, we give an additional estimate on the third derivatives of the finite-volume generating functionals. This result is not included in [88], since it has been proven afterwards. Its proof is very similar to the one of Proposition 7.4.2, albeit being much more computational.

Proposition 7.4.3 (Uniform boundedness of third derivatives)
Fix $\mathcal{E} \in C_0^0\left(\mathbb{R};\mathbb{R}^d\right)$ and $\beta_1, s_1, \vartheta_1, \lambda_1 \in \mathbb{R}^+$. Then,

$$\sup_{\substack{\beta\in(0,\beta_1],\ \vartheta\in[0,\vartheta_1],\ \lambda\in[0,\lambda_1]\\ \omega\in\Omega,\ s\in[-s_1,s_1],\ \mathcal{Z},\ \mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}\in\mathfrak{Z}_f}} \left|\partial_s^3 \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}\right| < \infty .$$

Proof: A straightforward computation implies that

$$\partial_s^3 \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} = \frac{1}{|\cup\mathcal{Z}|}\left(\varpi_s\left(\left(\Re^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\right)^3\right) - 3\varpi_s\left(\left(\Re^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\right)^2\right)\varpi_s\left(\Re^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\right) + 2\varpi_s\left(\Re^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\right)^3\right).$$

Since ϖ_s is a quasi-free state, note that, for any $x, y, u, v, z, w \in \mathbb{Z}^d$,

$$\varpi_s\left(a(\mathrm{e}_x)^* a\left(\mathrm{e}_y\right) a(\mathrm{e}_u)^* a(\mathrm{e}_v) a(\mathrm{e}_z)^* a(\mathrm{e}_w)\right) \tag{7.40}$$
$$= -\varpi_s\left(a(\mathrm{e}_x)^* a(\mathrm{e}_u)^* a(\mathrm{e}_z)^* a\left(\mathrm{e}_y\right) a(\mathrm{e}_v) a(\mathrm{e}_w)\right) \tag{7.41}$$
$$+\delta_{z,v}\varpi_s\left(a(\mathrm{e}_x)^* a\left(\mathrm{e}_y\right) a(\mathrm{e}_u)^* a(\mathrm{e}_w)\right) \tag{7.42}$$
$$-\delta_{u,y}\varpi_s\left(a(\mathrm{e}_x)^* a(\mathrm{e}_z)^* a(\mathrm{e}_v) a(\mathrm{e}_w)\right) \tag{7.43}$$
$$+\delta_{y,z}\varpi_s\left(a(\mathrm{e}_x)^* a(\mathrm{e}_u)^* a(\mathrm{e}_v) a(\mathrm{e}_w)\right), \tag{7.44}$$

where, by Definition 3.2.10,

$$\varpi_s\left(a(\mathrm{e}_x)^* a(\mathrm{e}_u)^* a(\mathrm{e}_z)^* a\left(\mathrm{e}_y\right) a(\mathrm{e}_v) a(\mathrm{e}_w)\right) \tag{7.45}$$
$$= \begin{vmatrix} \varpi_s\left(a^*(\mathrm{e}_x)a(\mathrm{e}_w)\right) & \varpi_s\left(a^*(\mathrm{e}_x)a(\mathrm{e}_v)\right) & \varpi_s\left(a^*(\mathrm{e}_x)a(\mathrm{e}_y)\right) \\ \varpi_s\left(a^*(\mathrm{e}_u)a(\mathrm{e}_w)\right) & \varpi_s\left(a^*(\mathrm{e}_u)a(\mathrm{e}_v)\right) & \varpi_s\left(a^*(\mathrm{e}_u)a(\mathrm{e}_y)\right) \\ \varpi_s\left(a^*(\mathrm{e}_z)a(\mathrm{e}_w)\right) & \varpi_s\left(a^*(\mathrm{e}_z)a(\mathrm{e}_v)\right) & \varpi_s\left(a^*(\mathrm{e}_z)a(\mathrm{e}_y)\right) \end{vmatrix}. \tag{7.46}$$

Therefore, by using (7.33) and (7.41)-(7.45) as well as Equation (7.7) and Definition 3.2.2 together with tedious computations,

$$\partial_s^3 \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} = \frac{1}{|\cup\mathcal{Z}|}\sum_{x,y,u,v,z,w\in\mathbb{Z}^d}\left\langle \mathrm{e}_x, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_y\right\rangle_{\mathfrak{h}}\left\langle \mathrm{e}_u, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_v\right\rangle_{\mathfrak{h}}\left\langle \mathrm{e}_z, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_w\right\rangle_{\mathfrak{h}}$$
$$\Big(\varpi_s\left(a^*(\mathrm{e}_x)a(\mathrm{e}_w)\right)\varpi_s\left(a\left(\mathrm{e}_y\right)a^*(\mathrm{e}_u)\right)\varpi_s\left(a(\mathrm{e}_v)a^*(\mathrm{e}_z)\right)+\varpi_s\left(a^*(\mathrm{e}_x)a\left(\mathrm{e}_y\right)\right)\varpi_s\left(a^*(\mathrm{e}_u)a(\mathrm{e}_w)\right)\varpi_s\left(a(\mathrm{e}_v)a^*(\mathrm{e}_z)\right)$$
$$+\varpi_s\left(a^*(\mathrm{e}_x)a(\mathrm{e}_w)\right)\varpi_s\left(a\left(\mathrm{e}_y\right)a^*(\mathrm{e}_z)\right)\varpi_s\left(a^*(\mathrm{e}_u)a(\mathrm{e}_v)\right)-\varpi_s\left(a^*(\mathrm{e}_x)a(\mathrm{e}_v)\right)\varpi_s\left(a\left(\mathrm{e}_y\right)a^*(\mathrm{e}_z)\right)\varpi_s\left(a^*(\mathrm{e}_u)a(\mathrm{e}_w)\right)$$
$$-2\varpi_s\left(a^*(\mathrm{e}_x)a(\mathrm{e}_v)\right)\varpi_s\left(a\left(\mathrm{e}_y\right)a^*(\mathrm{e}_u)\right)\varpi_s\left(a^*(\mathrm{e}_z)a(\mathrm{e}_w)\right)\Big).$$

Using elementary manipulations on the above sums, we then deduce that

$$\partial_s^3 \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} = \mathbf{K}_1 - \mathbf{K}_2 \tag{7.47}$$

with

$$\mathbf{K}_1 := \frac{1}{|\cup\mathcal{Z}|}\sum_{x,y,u,v,z,w\in\mathbb{Z}^d}\left\langle \mathrm{e}_x, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_y\right\rangle_{\mathfrak{h}}\left\langle \mathrm{e}_u, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_v\right\rangle_{\mathfrak{h}}\left\langle \mathrm{e}_z, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_w\right\rangle_{\mathfrak{h}} \tag{7.48}$$
$$\varpi_s\left(a^*\left(\mathrm{e}_x\right)a\left(\mathrm{e}_w\right)\right)\varpi_s\left(a\left(\mathrm{e}_y\right)a^*\left(\mathrm{e}_u\right)\right)\varpi_s\left(a\left(\mathrm{e}_v\right)a^*\left(\mathrm{e}_z\right)\right)$$

and

$$\mathbf{K}_2 := \frac{1}{|\cup\mathcal{Z}|}\sum_{x,y,u,v,z,w\in\mathbb{Z}^d}\left\langle \mathrm{e}_x, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_y\right\rangle_{\mathfrak{h}}\left\langle \mathrm{e}_u, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_v\right\rangle_{\mathfrak{h}}\left\langle \mathrm{e}_z, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_w\right\rangle_{\mathfrak{h}} \tag{7.49}$$
$$\varpi_s\left(a^*\left(\mathrm{e}_x\right)a\left(\mathrm{e}_v\right)\right)\varpi_s\left(a\left(\mathrm{e}_y\right)a^*\left(\mathrm{e}_z\right)\right)\varpi_s\left(a^*\left(\mathrm{e}_u\right)a\left(\mathrm{e}_w\right)\right) \tag{7.50}$$

By using the triangle inequality, we obtain that

$$\begin{aligned}|\mathbf{K}_1| \leq{}& \frac{1}{|\cup\mathcal{Z}|}\sum_{x,y,u,v,z,w\in\mathbb{Z}^d}\left|\left\langle \mathrm{e}_x, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_y\right\rangle_{\mathfrak{h}}\right|\left|\left\langle \mathrm{e}_u, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_v\right\rangle_{\mathfrak{h}}\right|\left|\left\langle \mathrm{e}_z, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_w\right\rangle_{\mathfrak{h}}\right|\\
&\left|\varpi_s\left(a^*\left(\mathrm{e}_x\right)a\left(\mathrm{e}_w\right)\right)\right|\left|\varpi_s(a(\mathrm{e}_y)a^*\left(\mathrm{e}_u\right))\right|\left|\varpi_s\left(a\left(\mathrm{e}_v\right)a^*\left(\mathrm{e}_z\right)\right)\right|\\
\leq{}& \sup_{z,w\in\mathbb{Z}^d}\left|\left\langle \mathrm{e}_z, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_w\right\rangle_{\mathfrak{h}}\right|\sup_{u\in\mathbb{Z}^d}\sum_{v\in\mathbb{Z}^d}\left|\left\langle \mathrm{e}_u, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_v\right\rangle_{\mathfrak{h}}\right|\frac{1}{|\cup\mathcal{Z}|}\sum_{x,y\in\mathbb{Z}^d}\left|\left\langle \mathrm{e}_x, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathrm{e}_y\right\rangle_{\mathfrak{h}}\right|\\
&\sup_{x\in\mathbb{Z}^d}\sum_{w\in\mathbb{Z}^d}\left|\varpi_s\left(a^*\left(\mathrm{e}_x\right)a\left(\mathrm{e}_w\right)\right)\right|\sup_{y\in\mathbb{Z}^d}\sum_{u\in\mathbb{Z}^d}\left|\varpi_s\left(a\left(\mathrm{e}_y\right)a^*\left(\mathrm{e}_u\right)\right)\right|\sup_{v\in\mathbb{Z}^d}\sum_{z\in\mathbb{Z}^d}\left|\varpi_s\left(a\left(\mathrm{e}_v\right)a^*\left(\mathrm{e}_z\right)\right)\right|\end{aligned}$$

Similar to (7.34)-(7.38), we then infer from Lemma 7.3.1, Corollary 7.3.2 and Equation (7.39) that

$$\sup_{\substack{\beta\in(0,\beta_1],\ \vartheta\in[0,\vartheta_1],\ \lambda\in[0,\lambda_1]\\ \omega\in\Omega,\ s\in[-s_1,s_1],\ \mathcal{Z},\ \mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}\in\mathfrak{Z}_{\mathrm{f}}}}|\mathbf{K}_1| < \infty.$$

The absolute value $|\mathbf{K}_2|$ of the other term of $\partial_s^3 \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}$ (see (7.47)-(7.49)) can be bounded exactly in the same way. By the triangle inequality, this concludes the proof. ■

The local generating functionals (7.23) can be approximately decomposed into boxes of fixed volume: By using the boxes (4.8), for any subset $\Lambda\subset\mathbb{Z}^d$ and $\ell\in\mathbb{N}$, we define the ℓ–th box decomposition $\mathcal{Z}^{(\Lambda,\ell)}$ of Λ by

$$\mathcal{Z}^{(\Lambda,\ell)} := \left\{\Lambda_\ell + (2\ell+1)\,x : x\in\mathbb{Z}^d \text{ with } (\Lambda_\ell + (2\ell+1)\,x)\subset\Lambda\right\}\in\mathfrak{Z}.$$

Then, we get the following assertion:

Proposition 7.4.4 (Box decomposition of generating functions)
Fix $n\in\mathbb{N}$ and $\beta_1,\lambda_1,\vartheta_1\in\mathbb{R}^+$. Then,

$$\lim_{\ell\to\infty}\limsup_{L_\tau\geq L_\varrho\geq L\to\infty}\left|\mathrm{J}^{(\omega,\mathcal{E})}_{\{\Lambda_\ell\},\{\Lambda_{L_\varrho}\},\{\Lambda_{L_\tau}\}} - \frac{1}{\left|\mathcal{Z}^{(\Lambda_L,\ell)}\right|}\sum_{Z\in\mathcal{Z}^{(\Lambda_L,\ell)}}\mathrm{J}^{(\omega,\mathcal{E})}_{\{Z\},\{Z\},\{Z\}}\right| = 0,$$

uniformly with respect to $\beta \in \left[0, \beta_1\right]$, $\vartheta \in [0, \vartheta_1]$, $\lambda \in [0, \lambda_1]$, $\omega \in \Omega$ *and* $\mathcal{E}$ *in any bounded set of* $C_0^\infty([-n, n]; \mathbb{R}^d)$.

The proof of this statement is divided in a series of Lemmata:

Lemma 7.4.5 (Box decomposition of generating functions – I)
Fix $\beta_1, \lambda_1, \vartheta_1 \in \mathbb{R}^+$. *Then,*

$$\limsup_{L_\tau \geq L_\varrho \geq L \to \infty} \left| g^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\},\{\Lambda_{L_\tau}\}} - g^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\backslash\Lambda_L,\Lambda_L\},\{\Lambda_{L_\tau}\}} \right| = 0,$$

uniformly with respect to $\beta \in \left[0, \beta_1\right]$, $\vartheta \in [0, \vartheta_1]$, $\lambda \in [0, \lambda_1]$, $\omega \in \Omega$ *and* $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$.

Proof: Fix all parameters of the lemma. By Lemma 7.2.3 (ii),

$$\left| g^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\},\{\Lambda_{L_\tau}\}} - g^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\backslash\Lambda_L,\Lambda_L\},\{\Lambda_{L_\tau}\}} \right| \leq \frac{\beta}{|\Lambda_L|} \sup_{\alpha\in[0,1]} \sup_{u\in[-1/2,1/2]} \left\| \mathrm{e}^{u\beta\langle \mathrm{A}, h_\alpha \mathrm{A}\rangle} \langle \mathrm{A}, (h_1 - h_0)\, \mathrm{A}\rangle\, \mathrm{e}^{-u\beta\langle \mathrm{A}, h_\alpha \mathrm{A}\rangle} \right\|_{\mathcal{U}},$$

where

$$h_\alpha := \alpha h^{(\omega)}_{\{\Lambda_{L_\varrho}\}} + (1-\alpha)\, h^{(\omega)}_{\{\Lambda_{L_\varrho}\backslash\Lambda_L,\Lambda_L\}}, \qquad \alpha \in [0,1]\,.$$

By using estimates similar to (7.28), we get

$$\begin{aligned} \left| g^{(\omega,\mathcal{E})}_{\{\Lambda_\ell\},\{\Lambda_{L_\varrho}\},\{\Lambda_{L_\tau}\}} - g^{(\omega,\mathcal{E})}_{\{\Lambda_\ell\},\{\Lambda_{L_\varrho}\backslash\Lambda_L,\Lambda_L\},\{\Lambda_{L_\tau}\}} \right| &\leq \frac{\beta \mathrm{e}^{\beta(\lambda+2d)(1+\vartheta)}}{|\Lambda_L|} \sum_{x,y\in\mathbb{Z}^d} \left| \left\langle \mathfrak{e}_x, (h_1 - h_0)\, \mathfrak{e}_y \right\rangle_{\mathfrak{h}} \right| \\ &\leq 4d\,(1+\vartheta)\,\beta \mathrm{e}^{\beta(\lambda+2d)(1+\vartheta)} \frac{1}{|\Lambda_L|} \sum_{z\in\cup\partial_{\Lambda_{L_\varrho}}(\Lambda_L)} 1. \end{aligned} \tag{7.51}$$

See (7.19). Since

$$\limsup_{L_\varrho \geq L \to \infty} \frac{1}{|\Lambda_L|} \sum_{z\in\cup\partial_{\Lambda_{L_\varrho}}(\Lambda_L)} 1 = 0,$$

the assertion follows. ∎

Lemma 7.4.6 (Box decomposition of generating functions – II)
Fix $n \in \mathbb{N}$ *and* $\vartheta_1, \lambda_1 \in \mathbb{R}^+$. *Then,*

$$\lim_{\ell\to\infty} \limsup_{L_\tau \geq L_\rho \geq L \to \infty} \left| g^{(\omega,\mathcal{E})}_{\{\Lambda_\ell\},\{\Lambda_{L_\varrho}\backslash\Lambda_L,\Lambda_L\},\{\Lambda_{L_\tau}\}} - g^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\backslash\Lambda_L,\Lambda_L\},\mathcal{Z}^{(\Lambda_L,\ell)}} \right| = 0,$$

uniformly with respect to $\vartheta \in [0, \vartheta_1]$, $\lambda \in [0, \lambda_1]$, $\omega \in \Omega$ *and* $\mathcal{E}$ *in any bounded set of* $C_0^0([-n, n]; \mathbb{R}^d)$.

Proof: Fix all parameters of the lemma, in particular $L_\tau \geq L_\rho \geq L \geq l$, $\omega \in \Omega$ and $\lambda \in [0, \lambda_1]$. By Lemma 7.2.3 (ii) and (7.7),

$$\left| g^{(\omega,\mathcal{E})}_{\{\Lambda_\ell\},\{\Lambda_{L_\varrho}\backslash\Lambda_L,\Lambda_L\},\{\Lambda_{L_\tau}\}} - g^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\backslash\Lambda_L,\Lambda_L\},\mathcal{Z}^{(\Lambda_L,\ell)}} \right|$$
$$\leq \frac{1}{|\Lambda_\ell|} \sup_{\alpha\in[0,1]} \sup_{u\in[-1/2,1/2]} \left\| \mathrm{e}^{u\langle \mathrm{A},K_\alpha \mathrm{A}\rangle} \langle \mathrm{A}, (K_1 - K_0)\, \mathrm{A}\rangle \, \mathrm{e}^{-u\langle \mathrm{A},K_\alpha \mathrm{A}\rangle} \right\|_{\mathcal{U}},$$

where

$$K_\alpha := \alpha K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\tau}\}} + (1-\alpha)\, K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\mathcal{Z}^{(\Lambda_L,\ell)}}, \qquad \alpha \in [0,1]\,.$$

Like in the proof of Lemma 7.4.5, by (7.7) and Lemma 7.3.3,

$$\left| g^{(\omega,\mathcal{E})}_{\{\Lambda_\ell\},\{\Lambda_{L_\varrho}\backslash\Lambda_L,\Lambda_L\},\{\Lambda_{L_\tau}\}} - g^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\backslash\Lambda_L,\Lambda_L\},\mathcal{Z}^{(\Lambda_L,\ell)}} \right| \tag{7.52}$$
$$\leq D_{7.3.3} \left(\int_{\mathbb{R}} \|\mathcal{E}(\alpha)\|_{\mathbb{R}^d}\, \alpha^2 \mathrm{e}^{2|\alpha\eta|} \mathrm{d}\alpha \right) \mathrm{e}^{\sup_{\alpha\in[0,1]} \|K_\alpha\|_{\mathcal{B}(\mathfrak{h})}} \tag{7.53}$$
$$\times \frac{1}{|\Lambda_L|} \left(\sum_{x\in\Lambda_L} \sum_{z\in\Lambda_{L_\tau}\backslash\cup\mathcal{Z}^{(\Lambda_L,\ell)}} \mathrm{e}^{-\frac{\mu_\eta}{2}|x-z|} + \left(\sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-\frac{\mu_\eta}{2}|z|} \right) \sum_{x\in\cup\partial_{\Lambda_{L_\tau}}(\mathcal{Z}^{(\Lambda_L,\ell)})} 1 \right). \tag{7.54}$$

By Lemmata 7.2.2 and 7.3.1, for any $n \in \mathbb{N}$, observe that the operator norms of K_α is uniformly bounded for $\alpha \in [0,1]$, $\vartheta \in [0, \vartheta_1]$, $\lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $L, L_\tau, \ell \in \mathbb{N}$ and $\mathcal{E}$ in any bounded set of $C_0^\infty([-n,n];\mathbb{R}^d)$. Note additionally that

$$\limsup_{L_\tau \geq L \to \infty} \frac{1}{|\Lambda_L|} \sum_{x\in\Lambda_L} \sum_{z\in\Lambda_{L_\tau}\backslash\cup\mathcal{Z}^{(\Lambda_L,\ell)}} \mathrm{e}^{-\frac{\mu_\eta}{2}|x-z|} = 0,$$

whereas

$$\limsup_{L_\tau \geq L \to \infty} \frac{1}{|\Lambda_L|} \sum_{x\in\cup\partial_{\Lambda_{L_\tau}}(\mathcal{Z}^{(\Lambda_L,\ell)})} 1 = \mathcal{O}\left(\ell^{-1}\right).$$

From these last observations combined with (7.52), the assertion follows. ∎

Lemma 7.4.7 (Box decomposition of generating functions – III)
Fix $\beta_1, \vartheta_1, \lambda_1 \in \mathbb{R}^+$. Then,

$$\lim_{\ell\to\infty} \limsup_{L_\tau \geq L_\varrho \geq L \to \infty} \left| g^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\backslash\Lambda_L,\Lambda_L\},\mathcal{Z}^{(\Lambda_L,\ell)}} - g^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\backslash\Lambda_L\}\cup\mathcal{Z}^{(\Lambda_L,\ell)},\mathcal{Z}^{(\Lambda_L,\ell)}} \right| = 0,$$

uniformly with respect to $\beta \in \left[0, \beta_1\right]$, $\vartheta \in [0, \vartheta_1]$, $\lambda \in [0, \lambda_1]$, $\omega \in \Omega$ and $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$.

Proof: This lemma is proven exaclty in the same way as Lemmata 7.4.5 and 7.4.6: Fix all parameters of the lemma and observe that

$$\begin{aligned}&\left|\left\langle \mathrm{e}_x, \left(h^{(\omega)}_{\{\Lambda_{L_\varrho}\backslash\Lambda_L,\Lambda_L\}} - h^{(\omega)}_{\{\Lambda_{L_\varrho}\backslash\Lambda_L\}\cup\mathcal{Z}^{(\Lambda_L,\ell)}}\right)\mathrm{e}_y\right\rangle_{\mathfrak{h}}\right| \\ \leq\ & (1+\vartheta)\sum_{z_3,z_4\in\Lambda_L\backslash\cup\mathcal{Z}^{(\Lambda_L,\ell)}\ :\ |z_3-z_4|=1}\delta_{z_3,y}\delta_{z_4,x} + \lambda\sum_{z_3\in\Lambda_L\backslash\cup\mathcal{Z}^{(\Lambda_L,\ell)}}\delta_{z_3,x}\delta_{z_3,y} \\ &+ (1+\vartheta)\sum_{Z\in\mathcal{Z}^{(\Lambda_L,\ell)}}\sum_{\{z_3,z_4\}\in\partial_{\Lambda_L}(Z)}\left(\delta_{z_3,y}\delta_{z_4,x}+\delta_{z_4,y}\delta_{z_3,x}\right).\end{aligned}$$

See (7.19). Then, similar to (7.51), we get the bound

$$\begin{aligned}&\left|g^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\backslash\Lambda_L,\Lambda_L\},\mathcal{Z}^{(\Lambda_L,\ell)}} - g^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\backslash\Lambda_L\}\cup\mathcal{Z}^{(\Lambda_L,\ell)},\mathcal{Z}^{(\Lambda_L,\ell)}}\right| \\ &\qquad\leq (4d+\lambda)(1+\vartheta)\beta\mathrm{e}^{\beta(\lambda+2d)(1+\vartheta)}\frac{1}{|\Lambda_L|}\left(\sum_{z\in\Lambda_L\backslash\cup\mathcal{Z}^{(\Lambda_L,\ell)}}1 + \sum_{Z\in\mathcal{Z}^{(\Lambda_L,\ell)}}\sum_{z\in\cup\partial_{\Lambda_L}(Z)}1\right),\end{aligned}$$

where

$$\limsup_{L\to\infty}\frac{1}{|\Lambda_L|}\left(\sum_{z\in\Lambda_L\backslash\cup\mathcal{Z}^{(\Lambda_L,\ell)}}1 + \sum_{Z\in\mathcal{Z}^{(\Lambda_L,\ell)}}\sum_{z\in\cup\partial_{\Lambda_L}(Z)}1\right) = \mathcal{O}\left(\ell^{-1}\right).$$

■

Lemma 7.4.8 (Box decomposition of generating functions – IV)
Fix $n\in\mathbb{N}$ and $\vartheta_1\in\mathbb{R}^+$. Then,

$$\lim_{\ell\to\infty}\limsup_{L_\tau\geq L_\varrho\geq L\to\infty}\left|g^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\backslash\Lambda_L\}\cup\mathcal{Z}^{(\Lambda_L,\ell)},\mathcal{Z}^{(\Lambda_L,\ell)}} - g^{(\omega,\mathcal{E})}_{\mathcal{Z}^{(\Lambda_L,\ell)},\{\Lambda_{L_\varrho}\backslash\Lambda_L\}\cup\mathcal{Z}^{(\Lambda_L,\ell)},\mathcal{Z}^{(\Lambda_L,\ell)}}\right| = 0,$$

uniformly with respect to $\beta\in\mathbb{R}^+$, $\vartheta\in[0,\vartheta_1]$, $\lambda\in\mathbb{R}_0^+$, $\omega\in\Omega$ and $\mathcal{E}$ in any bounded set of $C_0^0([-n,n];\mathbb{R}^d)$.

Proof: Fix all parameters of the lemma. Then, like for previous lemmata, we use again Lemma 7.2.3 (ii) and (7.7) to obtain the bound

$$\begin{aligned}&\left|g^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\backslash\Lambda_L\}\cup\mathcal{Z}^{(\Lambda_L,\ell)},\mathcal{Z}^{(\Lambda_L,\ell)}} - g^{(\omega,\mathcal{E})}_{\mathcal{Z}^{(\Lambda_L,\ell)},\{\Lambda_{L_\varrho}\backslash\Lambda_L\}\cup\mathcal{Z}^{(\Lambda_L,\ell)},\mathcal{Z}^{(\Lambda_L,\ell)}}\right| \\ &\qquad\leq\frac{1}{|\Lambda_L|}\sup_{\alpha\in[0,1]}\sup_{u\in[-1/2,1/2]}\left\|\mathrm{e}^{u\langle \mathrm{A},K_\alpha\mathrm{A}\rangle}\langle\mathrm{A},(K_1-K_0)\,\mathrm{A}\rangle\,\mathrm{e}^{-u\langle\mathrm{A},K_\alpha\mathrm{A}\rangle}\right\|_{\mathcal{U}},\end{aligned}$$

where

$$K_\alpha := \alpha K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\mathcal{Z}^{(\Lambda_L,\ell)}} + (1-\alpha)\,K^{(\omega,\mathcal{E})}_{\mathcal{Z}^{(\Lambda_L,\ell)},\mathcal{Z}^{(\Lambda_L,\ell)}},\qquad \alpha\in[0,1].$$

Therefore, by Lemmata 7.2.2, 7.3.1 and 7.3.4, the assertion follows. ■

We are now in a position to prove Proposition 7.4.4:

Proof: Fix all parameters of Proposition 7.4.4. By Lemmata 7.4.5-7.4.8,

$$\limsup_{L_\tau \geq L_\varrho \geq L \to \infty} \left| \mathrm{J}^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\},\{\Lambda_{L_\tau}\}} - \mathrm{J}^{(\omega,\mathcal{E})}_{\mathcal{Z}^{(\Lambda_L,\ell)},\{\Lambda_{L_\varrho}\backslash\Lambda_L\}\cup\mathcal{Z}^{(\Lambda_L,\ell)},\mathcal{Z}^{(\Lambda_L,\ell)}} \right| = 0, \tag{7.55}$$

uniformly with respect to $\beta \in \left[0, \beta_1\right]$, $\vartheta \in [0, \vartheta_1]$, $\lambda \in [0, \lambda_1]$, $\omega \in \Omega$ and $\mathcal{E}$ in any bounded set of $C_0^0([-n, n]; \mathbb{R}^d)$. To conclude the proof, observe that

$$\mathrm{J}^{(\omega,\mathcal{E})}_{\mathcal{Z}^{(\Lambda_L,\ell)},\{\Lambda_{L_\varrho}\backslash\Lambda_L\}\cup\mathcal{Z}^{(\Lambda_L,\ell)},\mathcal{Z}^{(\Lambda_L,\ell)}} = \mathrm{J}^{(\omega,\mathcal{E})}_{\mathcal{Z}^{(\Lambda_L,\ell)},\mathcal{Z}^{(\Lambda_L,\ell)},\mathcal{Z}^{(\Lambda_L,\ell)}} = \frac{1}{\left|\mathcal{Z}^{(\Lambda_L,\ell)}\right|} \sum_{Z \in \mathcal{Z}^{(\Lambda_L,\ell)}} \mathrm{J}^{(\omega,\mathcal{E})}_{\{Z\},\{Z\},\{Z\}}. \tag{7.56}$$

This follows from the fact that the tracial state tr is a product of single-site states. See, for instance, [21]. ■

7.5 Akcoglu–Krengel ergodic theorem and existence of generating functions

For convenience, we shortly recall the Akcoglu–Krengel ergodic theorem. We restrict ourselves to *additive* processes associated with the probability space $(\Omega, \mathfrak{A}_\Omega, \mathfrak{a}_\Omega)$ defined in Section 4.1, even if the Akcoglu–Krengel ergodic theorem holds for superadditive or subadditive ones (cf. [37, Definition VI.1.6]).

Definition 7.5.1 (Additive processes associated with random variables)
$\{\mathfrak{F}^{(\omega)}(\Lambda)\}_{\Lambda\in\mathcal{P}_f(\mathbb{Z}^d)}$ *is an additive process associated with the probability space* $(\Omega, \mathfrak{A}_\Omega, \mathfrak{a}_\Omega)$ *if:*
(i) the map $\omega \mapsto \mathfrak{F}^{(\omega)}(\Lambda)$ *is bounded and measurable with respect to the σ–algebra* $\mathfrak{A}_\Omega$ *for any* $\Lambda \in \mathcal{P}_f(\mathbb{Z}^d)$.
(ii) For all disjoint $\Lambda_1, \Lambda_2 \in \mathcal{P}_f(\mathbb{Z}^d)$,

$$\mathfrak{F}^{(\omega)}(\Lambda_1 \cup \Lambda_2) = \mathfrak{F}^{(\omega)}(\Lambda_1) + \mathfrak{F}^{(\omega)}(\Lambda_2) , \qquad \omega \in \Omega .$$

(iii) For all $\Lambda \in \mathcal{P}_f(\mathbb{Z}^d)$ *and any space shift* $x \in \mathbb{Z}^d$,

$$\mathbb{E}\left[\mathfrak{F}^{(\cdot)}(\Lambda)\right] = \mathbb{E}\left[\mathfrak{F}^{(\cdot)}(x + \Lambda)\right] . \tag{7.57}$$

Recall that $\mathbb{E}[\,\cdot\,]$ *is the expectation value associated with the distribution* $\mathfrak{a}_\Omega$.

We now define *regular* sequences (cf. [37, Remark VI.1.8]) as follows:

Definition 7.5.2 (Regular sequences)
The family $\{\Lambda^{(L)}\}_{L\in\mathbb{R}^+} \subset \mathcal{P}_f(\mathbb{Z}^d)$ of non–decreasing (possibly non–cubic) boxes of $\mathbb{Z}^d$ is a regular sequence if there is a finite constant $D \in (0,1]$ and a diverging sequence $\{\ell_L\}_{L\in\mathbb{R}^+}$ such that $\Lambda^{(L)} \subset \Lambda_{\ell_L}$ and $0 < |\Lambda_{\ell_L}| \leq D|\Lambda^{(L)}|$ for all $L \geq 1$. Here, $\{\Lambda_\ell\}_{\ell\in\mathbb{R}^+}$ is the sequence of boxes defined by (4.8).

Then, the form of Akcoglu–Krengel ergodic theorem we use in the sequel is the lattice version of [37, Theorem VI.1.7, Remark VI.1.8] for additive processes associated with the probability space $(\Omega, \mathfrak{A}_\Omega, \mathfrak{a}_\Omega)$:

Theorem 7.5.1 (Akcoglu–Krengel ergodic theorem)
Let $\{\mathfrak{F}^{(\omega)}(\Lambda)\}_{\Lambda\in\mathcal{P}_f(\mathbb{Z}^d)}$ be an additive process. Then, for any regular sequence $\{\Lambda^{(L)}\}_{L\in\mathbb{R}^+} \subset \mathcal{P}_f(\mathbb{Z}^d)$, there is a measurable subset $\tilde{\Omega} \subset \Omega$ of full measure such that, for all $\omega \in \tilde{\Omega}$,

$$\lim_{L\to\infty} \left\{ \left|\Lambda^{(L)}\right|^{-1} \mathfrak{F}^{(\omega)}\left(\Lambda^{(L)}\right) \right\} = \mathbb{E}\left[\mathfrak{F}^{(\cdot)}(\{0\})\right] .$$

See also [45].

The Ackoglu–Krengel (superadditive) ergodic theorem, cornerstone of ergodic theory, generalizes the celebrated Birkhoff additive ergodic theorem. It is used to deduce, via Proposition 7.4.1, the following Corollary:

Corollary 7.5.3 (Akcoglu–Krengel ergodic theorem for generating functions)
There is a measurable subset $\tilde{\Omega} \subset \Omega$ of full measure such that, for all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \tilde{\Omega}$, $l \in \mathbb{N}$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$,

$$\lim_{L\to\infty} \frac{1}{\left|\mathcal{Z}^{(\Lambda_L,l)}\right|} \sum_{Z\in\mathcal{Z}^{(\Lambda_L,l)}} \mathrm{J}^{(\omega,\mathcal{E})}_{\{Z\},\{Z\},\{Z\}} = \mathbb{E}\left[\mathrm{J}^{(\cdot,\mathcal{E})}_{\{\Lambda_l\},\{\Lambda_l\},\{\Lambda_l\}}\right].$$

Proof: Fix $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $l \in \mathbb{N}$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$. For any $\Gamma \in \mathcal{P}_{\mathrm{f}}(\mathbb{Z}^d)$, let

$$\mathfrak{F}_l^{(\omega,\mathcal{E})}(\Gamma) := \sum_{x\in\Gamma} \mathrm{J}^{(\omega,\mathcal{E})}_{\{\Lambda_l+(2l+1)x\},\{\Lambda_l+(2l+1)x\},\{\Lambda_l+(2l+1)x\}}.$$

Then, if

$$\Lambda^{(L)} \equiv \Lambda^{(L,l)} := \left\{x \in \mathbb{Z}^d : (\Lambda_\ell + (2l+1)\,x) \subset \Lambda_\ell\right\} \subset \Lambda_\ell,$$

observe that

$$\left|\Lambda^{(L)}\right|^{-1} \mathfrak{F}_l^{(\omega,\mathcal{E})}\left(\Lambda^{(L)}\right) = \frac{1}{\left|\mathcal{Z}^{(\Lambda_L,l)}\right|} \sum_{Z\in\mathcal{Z}^{(\Lambda_L,l)}} \mathrm{J}^{(\omega,\mathcal{E})}_{\{Z\},\{Z\},\{Z\}}.$$

Therefore, since $\{\Lambda^{(L)}\}_{L\in\mathbb{R}^+}$ is clearly a regular sequence, by Theorem 7.5.1, for any $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $l \in \mathbb{N}$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$, there is a measurable subset $\hat{\Omega} \equiv \hat{\Omega}^{(\beta,\vartheta,\lambda,l,\mathcal{E},\vec{w})} \subset \Omega$ of full measure such that, for all $\omega \in \hat{\Omega}$,

$$\lim_{L\to\infty} \frac{1}{\left|\mathcal{Z}^{(\Lambda_L,l)}\right|} \sum_{Z\in\mathcal{Z}^{(\Lambda_L,l)}} \mathrm{J}^{(\omega,\mathcal{E})}_{\{Z\},\{Z\},\{Z\}} = \mathbb{E}\left[\mathrm{J}^{(\cdot,\mathcal{E})}_{\{\Lambda_l\},\{\Lambda_l\},\{\Lambda_l\}}\right].$$

Observe that, for any $n \in \mathbb{N}$, there is a countable dense set $\mathcal{D}_n \subset C_0^0(\mathbb{R};\mathbb{R}^d)$. Let $\mathbb{S}^{d-1}$ be a dense countable subset of the $(d-1)$-dimensional sphere. Hence, by Proposition 7.4.1, we arrive at the assertion for any realization $\omega \in \tilde{\Omega} \subset \Omega$, where

$$\tilde{\Omega} := \bigcap_{\vartheta,\lambda\in\mathbb{Q}\cap\mathbb{R}_0^+} \bigcap_{\beta\in\mathbb{Q}\cap\mathbb{R}^+} \bigcap_{\vec{w}\in\mathbb{S}^{d-1}} \bigcap_{n\in\mathbb{N}} \bigcap_{\mathcal{E}\in\mathcal{D}_n} \bigcap_{l\in\mathbb{N}} \hat{\Omega}^{(\beta,\vartheta,\lambda,l,\mathcal{E},\vec{w})} .$$

[Recall that any countable intersection of measurable sets of full measure has full measure].
■

Corollary 7.5.4 (Almost surely existence of generating functions)
Let $\tilde{\Omega} \subset \Omega$ be the measurable subset of Corollary 7.5.3. Then, for all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \tilde{\Omega}$, $l \in \mathbb{N}$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$,

$$\lim_{L\to\infty} \frac{1}{|\Lambda_L|} \mathbb{E}\left[\ln \varrho^{(\cdot)}\left(\mathrm{e}^{|\Lambda_L|\mathbb{I}_{\Lambda_L}^{(\cdot,\mathcal{E})}}\right)\right] = \lim_{L_\tau \geq L_\varrho \geq L\to\infty} \mathrm{J}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\},\{\Lambda_{L_\tau}\}}^{(\omega,\mathcal{E})} := \mathrm{J}^{(\mathcal{E})}.$$

For all $n \in \mathbb{N}$, the convergence is uniform with respect to $\beta, \vartheta, \lambda$ in compact sets, $\omega \in \tilde{\Omega}$, $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$ and $\mathcal{E}$ in any bounded set of $C_0^0([-n,n];\mathbb{R}^d)$.

Proof: By translation invariance of the distribution $\mathfrak{a}_\Omega$,

$$\mathbb{E}\left[\mathrm{J}_{\{\Lambda_l\},\{\Lambda_l\},\{\Lambda_l\}}^{(\cdot,\mathcal{E})}\right] = \mathbb{E}\left[\frac{1}{\left|\mathcal{Z}^{(\Lambda_L,l)}\right|} \sum_{Z\in\mathcal{Z}^{(\Lambda_L,l)}} \mathrm{J}_{\{Z\},\{Z\},\{Z\}}^{(\cdot,\mathcal{E})}\right].$$

Hence,

$$\left\{\mathbb{E}\left[\mathrm{J}_{\{\Lambda_l\},\{\Lambda_l\},\{\Lambda_l\}}^{(\cdot,\mathcal{E})}\right]\right\}_{l\in\mathbb{N}}$$

is a Cauchy sequence, by (7.55) and (7.56). By Proposition 7.4.4 and Corollary 7.5.3, there is a measurable subset $\tilde{\Omega} \subset \Omega$ of full measure such that, for all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \tilde{\Omega}$, $l \in \mathbb{N}$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$,

$$\lim_{L_\tau \geq L_\varrho \geq L\to\infty} \mathrm{J}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\},\{\Lambda_{L_\tau}\}}^{(\omega,\mathcal{E})} = \lim_{l\to\infty} \mathbb{E}\left[\mathrm{J}_{\{\Lambda_l\},\{\Lambda_l\},\{\Lambda_l\}}^{(\cdot,\mathcal{E})}\right].$$

For all $n \in \mathbb{N}$, the convergence is uniform with respect to $\beta, \vartheta, \lambda$ in compact sets, $\omega \in \tilde{\Omega}$, $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$ and $\mathcal{E}$ in any bounded set of $C_0^0([-n,n];\mathbb{R}^d)$. By (7.25), the assertion then follows. ■

Corollary 7.5.5 (Differentiability of generating functions)
Fix $\beta, \lambda, \vartheta \in \mathbb{R}^+$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$. For any $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$, the map $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ is a $C^2(\mathbb{R},\mathbb{R})$ function.

Proof: Take any
$$\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$$
and $\omega \in \tilde{\Omega}$. See Corollary 7.5.4. Then, for any $s \in \mathbb{R}$,
$$\mathrm{J}^{(s\mathcal{E})} = \lim_{L_\tau \geq L_\varrho \geq L \to \infty} \mathrm{J}^{(\omega,s\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\},\{\Lambda_{L_\tau}\}}.$$
By Proposition 7.4.2, Proposition 7.4.3, the mean value theorem and the (Arzelà–) Ascoli theorem [54, Theorem A5], there are three sequences $\{L_\tau^{(n)}\}_{n\in\mathbb{N}}$, $\{L_\varrho^{(n)}\}_{n\in\mathbb{N}}$, $\{L^{(n)}\}_{n\in\mathbb{N}} \subset \mathbb{R}_0^+$, with $L_\tau^{(n)} \geq L_\varrho^{(n)} \geq L^{(n)}$, such that the maps
$$s \mapsto \mathrm{J}^{(\omega,s\mathcal{E})}_{\{\Lambda_{L^{(n)}}\},\{\Lambda_{L_\varrho^{(n)}}\},\{\Lambda_{L_\tau^{(n)}}\}}, \quad s \mapsto \partial_s \mathrm{J}^{(\omega,s\mathcal{E})}_{\{\Lambda_{L^{(n)}}\},\{\Lambda_{L_\varrho^{(n)}}\},\{\Lambda_{L_\tau^{(n)}}\}} \quad \text{and} \quad s \mapsto \partial_s^2 \mathrm{J}^{(\omega,s\mathcal{E})}_{\{\Lambda_{L^{(n)}}\},\{\Lambda_{L_\varrho^{(n)}}\},\{\Lambda_{L_\tau^{(n)}}\}}$$
converge uniformly for s in any compact set of $\mathbb{R}$. In particular, the map $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ from $\mathbb{R}$ to itself is a C^2-function with
$$\partial_s \mathrm{J}^{(s\mathcal{E})} = \lim_{L_\tau \geq L_\varrho \geq L \to \infty} \partial_s \mathrm{J}^{(\omega,s\mathcal{E})}_{\{\Lambda_{L^{(n)}}\},\{\Lambda_{L_\varrho^{(n)}}\},\{\Lambda_{L_\tau^{(n)}}\}} = \lim_{L\to\infty} \left(\frac{\varrho^{(\omega)}\left(\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})} \mathrm{e}^{s|\Lambda_L|\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}}\right)}{\varrho^{(\omega)}\left(\mathrm{e}^{s|\Lambda_L|\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}}\right)} \right)$$
and
$$\begin{aligned}\partial_s^2 \mathrm{J}^{(s\mathcal{E})} &= \lim_{L_\tau \geq L_\varrho \geq L \to \infty} \partial_s^2 \mathrm{J}^{(\omega,s\mathcal{E})}_{\{\Lambda_{L^{(n)}}\},\{\Lambda_{L_\varrho^{(n)}}\},\{\Lambda_{L_\tau^{(n)}}\}} \\ &= \lim_{L\to\infty} |\Lambda_L| \left(\frac{\varrho^{(\omega)}\left(\left(\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}\right)^2 \mathrm{e}^{s|\Lambda_L|\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}}\right) \varrho^{(\omega)}\left(\mathrm{e}^{s|\Lambda_L|\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}}\right) - \left(\varrho^{(\omega)}\left(\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})} \mathrm{e}^{s|\Lambda_L|\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}}\right)\right)^2}{\left(\varrho^{(\omega)}\left(\mathrm{e}^{s|\Lambda_L|\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}}\right)\right)^2} \right).\end{aligned}$$
■

In particular, for $s = 0$,
$$\partial_s \mathrm{J}^{(s\mathcal{E})}|_{s=0} = \lim_{L\to\infty} \mathbb{E}\left[\varrho^{(\omega)}\left(\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}\right)\right] = \lim_{L\to\infty} \varrho^{(\omega)}\left(\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}\right) \tag{7.58}$$
and
$$\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} = \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \mathbb{E}\left[\left(\varrho^{(\omega)}\left(\left(\mathfrak{K}^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\right)^2\right) - \left(\varrho^{(\omega)}\left(\mathfrak{K}^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\right)\right)^2\right)\right] \tag{7.59}$$
$$= \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \left(\varrho^{(\omega)}\left(\left(\mathfrak{K}^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\right)^2\right) - \left(\varrho^{(\omega)}\left(\mathfrak{K}^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\right)\right)^2\right). \tag{7.60}$$
(See, e.g., Proposition 7.4.2 with Lebesgue's dominated convergence theorem.) Observe that by Equations (7.58)-(7.60), $\partial_s \mathrm{J}^{(s\mathcal{E})}|_{s=0}$ corresponds to the macroscopic current density while $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0}$ is related to the current fluctuations.

7.6 Discussion on the positiveness of $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0}$

We discuss some necessary conditions to obtain

$$\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} \neq 0, \tag{7.61}$$

which appears in Proposition 5.4.1 (ii). By (7.31), (7.32) and the CAR (3.12) together with straightforward computations, one obtains from (5.18) that, for all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$,

$$\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} = \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \mathbb{E}\left[\mathrm{Tr}_{\mathfrak{h}}\left(K_{\{\Lambda_L\},\{\mathbb{Z}^d\}}^{(\omega,\mathcal{E})} \frac{1}{1+\mathrm{e}^{-\beta h^{(\omega)}}} K_{\{\Lambda_L\},\{\mathbb{Z}^d\}}^{(\omega,\mathcal{E})} \frac{1}{1+\mathrm{e}^{\beta h^{(\omega)}}}\right)\right] \tag{7.62}$$

with $\mathrm{Tr}_{\mathfrak{h}}$ being the trace on $\mathfrak{h} := \ell^2(\mathbb{Z}^d)$. Recall that $K_{\{\Lambda_L\},\{\mathbb{Z}^d\}}^{(\omega,\mathcal{E})}$ is defined by (7.10), that is in this case,

$$K_{\{\Lambda_L\},\{\mathbb{Z}^d\}}^{(\omega,\mathcal{E})} := \sum_{k,q=1}^{d} w_k \int_{-\infty}^{0} \{\mathcal{E}(\alpha)\}_q \left(\delta_{k,q} \mathbf{M}_k^{(L,\omega)} + \int_0^{-\alpha} \mathbf{N}_{\gamma,q,k}^{(L,\omega)} \mathrm{d}\gamma\right) \mathrm{d}\alpha, \tag{7.63}$$

where, for any $k, q \in \{1,\ldots,d\}$, $\gamma \in \mathbb{R}$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$ and $L \in \mathbb{R}^+$,

$$\mathbf{M}_k^{(L,\omega)} := \sum_{x,x+e_k\in\Lambda_L} 2\Re\mathrm{e}\{S_{x+e_k,x}^{(\omega)}\} \tag{7.64}$$

$$\mathbf{N}_{\gamma,q,k}^{(L,\omega)} := \sum_{x,y,x+e_k,y+e_q\in\Lambda_L} 4i\left[\mathrm{e}^{-i\gamma h^{(\omega)}} \Im\mathrm{m}\{S_{y+e_q,y}^{(\omega)}\} \mathrm{e}^{i\gamma h^{(\omega)}}, \Im\mathrm{m}\{S_{x+e_k,x}^{(\omega)}\}\right] \tag{7.65}$$

with, for any $x, y \in \mathbb{Z}^d$ and $\psi \in \mathfrak{h}$,

$$S_{x,y}^{(\omega)} := \langle \mathfrak{e}_y, \Delta_{\omega,\vartheta} \mathfrak{e}_x \rangle_{\mathfrak{h}} P_{\{y\}} s_{y-x} P_{\{x\}} \quad \text{and} \quad (s_x \psi)(y) := \psi(x+y). \tag{7.66}$$

See (7.5)-(7.6). Therefore, in order to satisfy (7.61), one needs to prove that

$$\lim_{L\to\infty} \left\{\frac{1}{|\Lambda_L|} \left|\mathrm{Tr}_{\mathfrak{h}}\left(K_{\{\Lambda_L\},\{\mathbb{Z}^d\}}^{(\omega,\mathcal{E})} \frac{1}{1+\mathrm{e}^{-\beta h^{(\omega)}}} K_{\{\Lambda_L\},\{\mathbb{Z}^d\}}^{(\omega,\mathcal{E})} \frac{1}{1+\mathrm{e}^{\beta h^{(\omega)}}}\right)\right|\right\} \geq \varepsilon > 0$$

for some strictly positive constant $\varepsilon \in \mathbb{R}^+$. We start by an elementary observation:

Lemma 7.6.1 (Quantum fluctuations and the Hilbert-Schmidt norm of $K_{\{\Lambda_L\},\{\mathbb{Z}^d\}}^{(\omega,\mathcal{E})}$)
For all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$,

$$\mathrm{Tr}_{\mathfrak{h}}\left(K_{\{\Lambda_L\},\{\mathbb{Z}^d\}}^{(\omega,\mathcal{E})} \frac{1}{1+\mathrm{e}^{-\beta h^{(\omega)}}} K_{\{\Lambda_L\},\{\mathbb{Z}^d\}}^{(\omega,\mathcal{E})} \frac{1}{1+\mathrm{e}^{\beta h^{(\omega)}}}\right) \geq \frac{1}{\left(1+\mathrm{e}^{\beta(2d(2+\vartheta)+\lambda)}\right)^2} \mathrm{Tr}_{\mathfrak{h}}\left(\left(K_{\{\Lambda_L\},\{\mathbb{Z}^d\}}^{(\omega,\mathcal{E})}\right)^* K_{\{\Lambda_L\},\{\mathbb{Z}^d\}}^{(\omega,\mathcal{E})}\right)$$

with $\mathrm{Tr}_{\mathfrak{h}}$ being the trace on $\mathfrak{h} := \ell^2(\mathbb{Z}^d)$.

Proof: Fix all parameters of the lemma. By using functional calculus, $(1 + \mathrm{e}^{\pm\beta h^{(\omega)}})^{-1}$ are positive operators satisfying

$$\frac{1}{1+\mathrm{e}^{\pm\beta h^{(\omega)}}} \geq \frac{1}{1+\mathrm{e}^{\beta \sup_{\omega\in\Omega} \|h^{(\omega)}\|_{\mathcal{B}(\mathfrak{h})}}}\mathbf{1}_{\mathfrak{h}}$$

where, for any $\omega = (\omega_1, \omega_2) \in \Omega$, $\lambda, \vartheta \in \mathbb{R}_0^+$, by (4.7)

$$\|h^{(\omega)}\|_{\mathcal{B}(\mathfrak{h})} \leq \|\Delta_{\omega,\vartheta}\|_{\mathcal{B}(\mathfrak{h})} + \lambda\|\omega_1\|_{\mathcal{B}(\mathfrak{h})} \leq 2d\,(2+\vartheta) + \lambda. \tag{7.67}$$

Since $K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}$ is a self-adjoint operator (see (7.63)), it thus suffices to use the cyclicity of the trace to prove the lemma. ∎

The square of the Hilbert-Schmidt norm of $K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}$ is obviously equal to

$$\mathrm{Tr}_{\mathfrak{h}}\left(\left(K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\right)^* K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\right) = \sum_{z\in\mathbb{Z}^d} \left\|K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\mathfrak{e}_z\right\|^2_{\mathfrak{h}}$$

and, as a consequence, we need an explicit expression of the vectors

$$K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\mathfrak{e}_z \in \mathfrak{h}, \qquad z \in \mathbb{Z}^d\ .$$

This can be directly deduced from (7.63) together with the following assertion:

Lemma 7.6.2 (Explicit computations of $\mathbf{M}_k^{(L,\omega)}$ and $\mathbf{N}_{\gamma,q,k}^{(L,\omega)}$ on the canonical basis)
For all $k, q \in \{1, \ldots, d\}$, $\gamma \in \mathbb{R}$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$ and $L \geq 2$ and $z \in \Lambda_{L/2}$,

$$\mathbf{M}_k^{(L,\omega)}\mathfrak{e}_z = \langle \mathfrak{e}_{z-e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_z\rangle_{\mathfrak{h}}\mathfrak{e}_{z-e_k} + \langle \mathfrak{e}_{z+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_z\rangle_{\mathfrak{h}}\mathfrak{e}_{z+e_k}$$

and, in the limit $L \to \infty$,

$$\mathbf{N}_{\gamma,q,k}^{(L,\omega)}\mathfrak{e}_z = \sum_{x,y\in\mathbb{Z}^d} \zeta_{x,y,z}\mathfrak{e}_x + \mathbf{R}_{\gamma,q,k}^{(L,\omega)}\mathfrak{e}_z\ , \qquad \sum_{x,y\in\mathbb{Z}^d} \left|\zeta_{x,y,z}\right|^2 < \infty\ ,$$

with $\mathbf{R}_{\gamma,q,k}^{(L,\omega)} \in \mathcal{B}(\mathfrak{h})$ satisfying

$$\lim_{L\to\infty} \left\|\mathbf{R}_{\gamma,q,k}^{(L,\omega)}\right\|_{\mathcal{B}(\mathfrak{h})} = 0,$$

uniformly with respect to $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and ϑ,γ in compact sets of $\mathbb{R}_0^+$ and $\mathbb{R}^+$, respectively, and *where, for any* $x, y, z \in \mathbb{Z}^d$,

$$
\begin{aligned}
\zeta_{x,y,z} := {} & i(1+\vartheta\omega_2(\{x-e_k,x\}))(1+\vartheta\omega_2(\{y,y+e_q\}))\langle \mathfrak{e}_{x-e_k}, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_y, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_z\rangle_{\mathfrak{h}} \\
& - i(1+\vartheta\omega_2(\{x-e_k,x\}))(1+\vartheta\overline{\omega_2(\{y+e_q,y\})})\langle \mathfrak{e}_{x-e_k}, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_z\rangle_{\mathfrak{h}} \\
& - i(1+\vartheta\overline{\omega_2(\{x+e_k,x\})})(1+\vartheta\omega_2(\{y,y+e_q\}))\langle \mathfrak{e}_{x+e_k}, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_y, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_z\rangle_{\mathfrak{h}} \\
& + i(1+\vartheta\overline{\omega_2(\{x+e_k,x\})})(1+\vartheta\overline{\omega_2(\{y+e_q,y\})})\langle \mathfrak{e}_{x+e_k}, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_z\rangle_{\mathfrak{h}} \\
& - i(1+\vartheta\omega_2(\{y,y+e_q\}))(1+\vartheta\omega_2(\{z,z+e_k\}))\langle \mathfrak{e}_{y}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_{z+e_k}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_x, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} \\
& + i(1+\vartheta\omega_2(\{y,y+e_q\}))(1+\vartheta\overline{\omega_2(\{z,z-e_k\})})\langle \mathfrak{e}_{y}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_{z-e_k}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_x, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} \\
& + i(1+\vartheta\overline{\omega_2(\{y+e_q,y\})})(1+\vartheta\omega_2(\{z,z+e_k\}))\langle \mathfrak{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_{z+e_k}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_x, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y}\rangle_{\mathfrak{h}} \\
& - i(1+\vartheta\overline{\omega_2(\{y+e_q,y\})})(1+\vartheta\overline{\omega_2(\{z,z-e_k\})})\langle \mathfrak{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_{z-e_k}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_x, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y}\rangle_{\mathfrak{h}}.
\end{aligned}
$$

Proof: Fix in all the proof $k, q \in \{1, \ldots, d\}$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\gamma \in \mathbb{R}$, $L \geq 2$ and $z \in \Lambda_{L/2}$. Since, for any $x, y \in \mathbb{Z}^d$,

$$2\Re\mathrm{e}\{S_{x,y}^{(\omega)}\} = \langle \mathfrak{e}_y, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}} P_{\{y\}} s_{y-x} P_{\{x\}} + \langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}} P_{\{x\}} s_{x-y} P_{\{y\}}$$

we deduce from (7.64) and (7.66) that

$$
\begin{aligned}
\mathbf{M}_k^{(L,\omega)} &= \sum_{x,x+e_k\in\Lambda_L} \left(\delta_{z,x+e_k}\langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}}\mathfrak{e}_x + \delta_{z,x}\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}}\mathfrak{e}_{x+e_k}\right) \\
&= \mathbf{1}\left[(z-e_k)\in\Lambda_L\right]\langle \mathfrak{e}_{z-e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_z\rangle_{\mathfrak{h}}\mathfrak{e}_{z-e_k} + \mathbf{1}\left[z\in\Lambda_L\right]\langle \mathfrak{e}_{z+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_z\rangle_{\mathfrak{h}}\mathfrak{e}_{z+e_k}.
\end{aligned}
$$

If $z \in \Lambda_{L/2} \subseteq \Lambda_L$ and $L \geq 2$ then, obviously, $z, (z-e_k) \in \Lambda_L$ and the last equality yields the first assertion.

Since, for any $x, y \in \mathbb{Z}^d$,

$$2\Im\mathrm{m}\{S_{x,y}^{(\omega)}\} = i\left(\langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}} P_{\{x\}} s_{x-y} P_{\{y\}} - \langle \mathfrak{e}_y, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}} P_{\{y\}} s_{y-x} P_{\{x\}}\right),$$

we compute that

$$
\begin{aligned}
& 4i\left[\mathrm{e}^{-i\gamma h^{(\omega)}}\Im\mathrm{m}\{S_{y+e_q,y}^{(\omega)}\}\mathrm{e}^{i\gamma h^{(\omega)}}, \Im\mathrm{m}\{S_{x+e_k,x}^{(\omega)}\}\right] \\
={} & i\left(\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}} s_{e_k} P_{\{x\}} - \langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}} s_{-e_k} P_{\{x+e_k\}}\right) \\
& \times \mathrm{e}^{-i\gamma h^{(\omega)}}\left(\langle \mathfrak{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}} s_{e_q} P_{\{y\}} - \langle \mathfrak{e}_y, \Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} s_{-e_q} P_{\{y+e_q\}}\right)\mathrm{e}^{i\gamma h^{(\omega)}} \\
& - i\mathrm{e}^{-i\gamma h^{(\omega)}}\left(\langle \mathfrak{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}} s_{e_q} P_{\{y\}} - \langle \mathfrak{e}_y, \Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} s_{-e_q} P_{\{y+e_q\}}\right)\mathrm{e}^{i\gamma h^{(\omega)}} \\
& \times \left(\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}} s_{e_k} P_{\{x\}} - \langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}} s_{-e_k} P_{\{x+e_k\}}\right)
\end{aligned}
$$

for any $x, y \in \mathbb{Z}^d$, which is developed to obtain that

$$\begin{aligned}
&4i\left[\mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{Im}\{S^{(\omega)}_{y+e_q,y}\}\mathrm{e}^{i\gamma h^{(\omega)}}, \mathfrak{Im}\{S^{(\omega)}_{x+e_k,x}\}\right] \\
&= i\langle \mathrm{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathrm{e}_x\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathrm{e}_y\rangle_{\mathfrak{h}} s_{e_k}P_{\{x\}}\mathrm{e}^{-i\gamma h^{(\omega)}}s_{e_q}P_{\{y\}}\mathrm{e}^{i\gamma h^{(\omega)}} \\
&\quad - i\langle \mathrm{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathrm{e}_x\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y}, \Delta_{\omega,\vartheta}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}} s_{e_k}P_{\{x\}}\mathrm{e}^{-i\gamma h^{(\omega)}}s_{-e_q}P_{\{y+e_q\}}\mathrm{e}^{i\gamma h^{(\omega)}} \\
&\quad - i\langle \mathrm{e}_{x}, \Delta_{\omega,\vartheta}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathrm{e}_y\rangle_{\mathfrak{h}} s_{-e_k}P_{\{x+e_k\}}\mathrm{e}^{-i\gamma h^{(\omega)}}s_{e_q}P_{\{y\}}\mathrm{e}^{i\gamma h^{(\omega)}} \\
&\quad + i\langle \mathrm{e}_{x}, \Delta_{\omega,\vartheta}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y}, \Delta_{\omega,\vartheta}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}} s_{-e_k}P_{\{x+e_k\}}\mathrm{e}^{-i\gamma h^{(\omega)}}s_{-e_q}P_{\{y+e_q\}}\mathrm{e}^{i\gamma h^{(\omega)}} \\
&\quad - i\langle \mathrm{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathrm{e}_x\rangle_{\mathfrak{h}} \mathrm{e}^{-i\gamma h^{(\omega)}}s_{e_q}P_{\{y\}}\mathrm{e}^{i\gamma h^{(\omega)}}s_{e_k}P_{\{x\}} \\
&\quad + i\langle \mathrm{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x}, \Delta_{\omega,\vartheta}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}} \mathrm{e}^{-i\gamma h^{(\omega)}}s_{e_q}P_{\{y\}}\mathrm{e}^{i\gamma h^{(\omega)}}s_{-e_k}P_{\{x+e_k\}} \\
&\quad + i\langle \mathrm{e}_{y}, \Delta_{\omega,\vartheta}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathrm{e}_x\rangle_{\mathfrak{h}} \mathrm{e}^{-i\gamma h^{(\omega)}}s_{-e_q}P_{\{y+e_q\}}\mathrm{e}^{i\gamma h^{(\omega)}}s_{e_k}P_{\{x\}} \\
&\quad - i\langle \mathrm{e}_{y}, \Delta_{\omega,\vartheta}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x}, \Delta_{\omega,\vartheta}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}} \mathrm{e}^{-i\gamma h^{(\omega)}}s_{-e_q}P_{\{y+e_q\}}\mathrm{e}^{i\gamma h^{(\omega)}}s_{-e_k}P_{\{x+e_k\}} .
\end{aligned}$$

Using this last equality together with (7.65) and (7.66), we thus get that

$$\begin{aligned}
\mathbf{N}^{(L,\omega)}_{\gamma,q,k}\mathrm{e}_z = \sum_{x,y,x+e_k,y+e_q\in\Lambda_L} \Big\{ & i\langle \mathrm{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathrm{e}_x\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_x, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_y, \mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_z\rangle_{\mathfrak{h}}\mathrm{e}_{x+e_k} \\
& - i\langle \mathrm{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathrm{e}_x\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y}, \Delta_{\omega,\vartheta}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_x, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_{y}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_z\rangle_{\mathfrak{h}}\mathrm{e}_{x+e_k} \\
& - i\langle \mathrm{e}_{x}, \Delta_{\omega,\vartheta}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x+e_k}, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_y, \mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_z\rangle_{\mathfrak{h}}\mathrm{e}_{x} \\
& + i\langle \mathrm{e}_{x}, \Delta_{\omega,\vartheta}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y}, \Delta_{\omega,\vartheta}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x+e_k}, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_{y}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_z\rangle_{\mathfrak{h}}\mathrm{e}_{x} \\
& - i\delta_{x,z}\langle \mathrm{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathrm{e}_x\rangle_{\mathfrak{h}}\langle \mathrm{e}_y, \mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_{y+e_q} \\
& + i\delta_{x+e_k,z}\langle \mathrm{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x}, \Delta_{\omega,\vartheta}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle \mathrm{e}_y, \mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_{x}\rangle_{\mathfrak{h}}\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_{y+e_q} \\
& + i\delta_{x,z}\langle \mathrm{e}_{y}, \Delta_{\omega,\vartheta}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathrm{e}_x\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_{y} \\
& -i\delta_{x+e_k,z}\langle \mathrm{e}_{y}, \Delta_{\omega,\vartheta}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x}, \Delta_{\omega,\vartheta}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_{x}\rangle_{\mathfrak{h}}\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_{y} . \Big\}
\end{aligned}$$

By (4.13) and the inequality (7.12), all the sums are absolutly summable, uniformally with respect to $L \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}^+_0$ and ϑ,t in compact sets of $\mathbb{R}^+_0$ and $\mathbb{R}^+$, respectively. Therefore, in the limit $L \to \infty$, for any $z \in \Lambda_{L/2}$, there is an operator $\mathbf{R}^{(L,\omega)}_{\gamma,q,k} \in \mathcal{B}(\mathfrak{h})$ with vanishing operator norm as $L \to \infty$, uniformly with respect to $\omega \in \Omega$, $\lambda \in \mathbb{R}^+_0$ and ϑ,γ in compact sets of $\mathbb{R}^+_0$ and $\mathbb{R}^+$, respectively, such that

$$\mathbf{N}^{(L,\omega)}_{\gamma,q,k}\mathrm{e}_z = \left(\mathbf{N}^{(\infty,\omega)}_{\gamma,q,k} + \mathbf{R}^{(L,\omega)}_{\gamma,q,k}\right)\mathrm{e}_z ,$$

where

$$\begin{aligned}\mathbf{N}_{\gamma,q,k}^{(\infty,\omega)}\mathrm{e}_z : = \sum_{x,y\in\mathbb{Z}^d}\Big\{ & i\langle \mathrm{e}_{x+e_k},\Delta_{\omega,\vartheta}\mathrm{e}_x\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q},\Delta_{\omega,\vartheta}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_x,\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_y,\mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_z\rangle_{\mathfrak{h}}\mathrm{e}_{x+e_k}\\
&- i\langle \mathrm{e}_{x+e_k},\Delta_{\omega,\vartheta}\mathrm{e}_x\rangle_{\mathfrak{h}}\langle \mathrm{e}_y,\Delta_{\omega,\vartheta}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_x,\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q},\mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_z\rangle_{\mathfrak{h}}\mathrm{e}_{x+e_k}\\
&- i\langle \mathrm{e}_x,\Delta_{\omega,\vartheta}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q},\Delta_{\omega,\vartheta}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x+e_k},\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_y,\mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_z\rangle_{\mathfrak{h}}\mathrm{e}_x\\
&+ i\langle \mathrm{e}_x,\Delta_{\omega,\vartheta}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle \mathrm{e}_y,\Delta_{\omega,\vartheta}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x+e_k},\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q},\mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_z\rangle_{\mathfrak{h}}\mathrm{e}_x\\
&- i\delta_{x,z}\langle \mathrm{e}_{y+e_q},\Delta_{\omega,\vartheta}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x+e_k},\Delta_{\omega,\vartheta}\mathrm{e}_x\rangle_{\mathfrak{h}}\langle \mathrm{e}_y,\mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_{y+e_q}\\
&+ i\delta_{x+e_k,z}\langle \mathrm{e}_{y+e_q},\Delta_{\omega,\vartheta}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_x,\Delta_{\omega,\vartheta}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle \mathrm{e}_y,\mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_x\rangle_{\mathfrak{h}}\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_{y+e_q}\\
&+ i\delta_{x,z}\langle \mathrm{e}_y,\Delta_{\omega,\vartheta}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{x+e_k},\Delta_{\omega,\vartheta}\mathrm{e}_x\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q},\mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_y\\
&- i\delta_{x+e_k,z}\langle \mathrm{e}_y,\Delta_{\omega,\vartheta}\mathrm{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathrm{e}_x,\Delta_{\omega,\vartheta}\mathrm{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle \mathrm{e}_{y+e_q},\mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_x\rangle_{\mathfrak{h}}\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_y.\Big\}\end{aligned}$$

Now, we use (4.6) and

$$\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_w = \sum_{u\in\mathbb{Z}^d}\mathrm{e}_u\langle \mathrm{e}_u,\mathrm{e}^{-i\gamma h^{(\omega)}}\mathrm{e}_w\rangle_{\mathfrak{h}}$$

for any $w \in \mathbb{Z}^d$ together with elementary manipulations in each sum of $\mathbf{N}_{\gamma,q,k}^{(\infty,\omega)}$ to arrive at the assertion. ■

We are now in a position to show (7.61), at least for $|\gamma|, \vartheta \ll 1$, as a consequence of the next two lemmata:

Lemma 7.6.3 (Asymptotics for $|\gamma|, \vartheta \ll 1$)
For all $k, q \in \{1, \ldots, d\}$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\gamma \in \mathbb{R}$, $L \geq 2$ and $z \in \Lambda_{L/2}$,

$$\sum_{y\in\mathbb{Z}^d}\zeta_{z,y,z} = 2\Im\mathrm{m}\left\langle\left(s_{e_k}-s_{-e_k}\right)\mathrm{e}_z,\mathrm{e}^{-i\gamma h^{(\omega)}}\left(s_{e_q}-s_{-e_q}\right)\mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_z\right\rangle_{\mathfrak{h}} + \mathcal{O}(\vartheta), \qquad \text{as } \vartheta\to 0,$$

uniformly with respect to $\omega \in \Omega$ and γ, λ in compact sets of $\mathbb{R}_0^+$.

Proof: By Lemma 7.6.2 and (4.13), it suffices to show the assertion at $\vartheta = 0$. In fact, by Lemma 7.6.2 at $\vartheta = 0$, one directly computes that, for any $k, q \in \{1, \ldots, d\}$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\gamma \in \mathbb{R}$, $L \geq 2$ and $z \in \Lambda_{L/2}$,

$$\sum_{y\in\mathbb{Z}^d}\zeta_{z,y,z} = \sum_{y\in\mathbb{Z}^d}2\Im\mathrm{m}\langle \mathrm{e}_{z+e_k}-\mathrm{e}_{z-e_k},\mathrm{e}^{-i\gamma h^{(\omega)}}\left(\mathrm{e}_{y+e_q}-\mathrm{e}_{y-e_q}\right)\rangle_{\mathfrak{h}}\langle \mathrm{e}_y,\mathrm{e}^{i\gamma h^{(\omega)}}\mathrm{e}_z\rangle_{\mathfrak{h}},$$

from which we trivially deduce the assertion, by (7.66). ■

Lemma 7.6.4
For all $k,q \in \{1,\ldots,d\}$, $\vartheta,\lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $z \in \mathbb{Z}^d$ and $\gamma \in \mathbb{R}$,

$$2\mathfrak{Im}\left\langle \left(s_{e_k} - s_{-e_k}\right) \mathfrak{e}_z, \mathrm{e}^{-i\gamma h^{(\omega)}} \left(s_{e_q} - s_{-e_q}\right) \mathrm{e}^{i\gamma h^{(\omega)}} \mathfrak{e}_z \right\rangle_{\mathfrak{h}} = 2\gamma\lambda\delta_{k,q} \left\{2\omega_1(z) - \omega_1(z+e_k) - \omega_1(z-e_k)\right\} + \mathcal{O}\left(\gamma^2\right),$$

as $|\gamma| \to 0$, uniformly with respect to $\omega \in \Omega$ and ϑ,λ in compact sets of $\mathbb{R}_0^+$.

Proof: Fix all parameters of the lemma. By (7.67),

$$\mathrm{e}^{i\gamma h^{(\omega)}} = \mathbf{1}_{\mathfrak{h}} + \sum_{n\in\mathbb{N}} \frac{\left(i\gamma h^{(\omega)}\right)^n}{n!} = \mathbf{1}_{\mathfrak{h}} + i\gamma h^{(\omega)} + \mathcal{O}\left(\gamma^2\right), \qquad \text{as } |\gamma| \to 0,$$

uniformly with respect to $\omega \in \Omega$ and ϑ,λ in compact sets of $\mathbb{R}_0^+$. The assertion then follows by direct computations using (4.7), (7.66), and the last equality. ■

Lemma 7.6.5 (Lower bounds on the Hilbert-Schmidt norm of $K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}$)
Take $\vartheta,\lambda,T \in \mathbb{R}_0^+$, $T \in \mathbb{R}^+$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ with support in $[-T,0]$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$. If T,ϑ are sufficiently small then

$$\lim_{L\to\infty} \frac{1}{|\Lambda_L|} \mathbb{E}\left[\mathrm{Tr}_{\mathfrak{h}}\left(\left(K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\right)^* K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\right)\right] \geq \lambda^2 \mathbb{E}\left[\left|\int_{-\infty}^0 \left\langle w^{(\omega)}, \mathcal{E}(\alpha)\right\rangle_{\mathbb{R}^d} \alpha^2 \mathrm{d}\alpha\right|^2\right] + \mathcal{O}\left(\vartheta^2\right) + \mathcal{O}\left(T^4\right)$$

uniformly with respect to λ in compact sets of $\mathbb{R}_0^+$, where, for any $\omega \in \Omega$, $w^{(\omega)} := (w_1^{(\omega)},\ldots,w_d^{(\omega)}) \in \mathbb{R}^d$ is the random vector defined by

$$w_k^{(\omega)} := \left(2\omega_1(0) - \omega_1(e_k) - \omega_1(-e_k)\right) w_k, \qquad k \in \{1,\ldots,d\}. \tag{7.68}$$

Proof: Fix all parameters of the lemma. Take any $L \geq 2$. Note that

$$\frac{1}{|\Lambda_L|} \mathrm{Tr}_{\mathfrak{h}}\left(\left(K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\right)^* K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\right) \geq \sum_{z\in\Lambda_{L/2}} \left\|K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \mathfrak{e}_z\right\|_{\mathfrak{h}}^2 \geq \sum_{z\in\Lambda_{L/2}} \left|\left\langle \mathfrak{e}_z, K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \mathfrak{e}_z\right\rangle_{\mathfrak{h}}\right|^2. \tag{7.69}$$

If T,ϑ are sufficiently small then, by using (7.63)-(7.65) with Lemmata 7.6.2-7.6.4 and the ergodicity of the distribution $\mathfrak{a}_\Omega$ (see (4.2)), we deduce that

$$\lim_{L\to\infty} \mathbb{E}\left[\left|\left\langle \mathfrak{e}_z, K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \mathfrak{e}_z\right\rangle_{\mathfrak{h}}\right|^2\right] = \lambda^2 \mathbb{E}\left[\left|\int_{-\infty}^0 \left\langle w^{(\omega)}, \mathcal{E}(\alpha)\right\rangle_{\mathbb{R}^d} \alpha^2 \mathrm{d}\alpha\right|^2\right] + \mathcal{O}\left(\vartheta^2\right) + \mathcal{O}\left(T^4\right) \tag{7.70}$$

uniformly with respect to λ in compact sets of $\mathbb{R}_0^+$. By (7.69), the assertion then follows. ∎

By combining Lemmata 7.6.1 and 7.6.5 with (7.62), we directly obtain that, for any $\vartheta, \lambda, T \in \mathbb{R}_0^+$, $T, \beta \in \mathbb{R}^+$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ with support in $[-T,0]$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$,

$$\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} \geq \frac{1}{2\left(1+\mathrm{e}^{\beta(2d(2+\vartheta)+\lambda)}\right)^2}\left(\lambda^2 \mathbb{E}\left[\left|\int_{-\infty}^0 \left\langle w^{(\omega)}, \mathcal{E}(\alpha)\right\rangle_{\mathbb{R}^d} \alpha^2 \mathrm{d}\alpha\right|^2\right] + \mathcal{O}\left(\vartheta^2\right) + \mathcal{O}\left(T^4\right)\right) \tag{7.71}$$

provided that T, ϑ are sufficiently small. In particular, if

$$\mathbb{E}\left[\left|\int_{-\infty}^0 \left\langle w^{(\omega)}, \mathcal{E}(\alpha)\right\rangle_{\mathbb{R}^d} \alpha^2 \mathrm{d}\alpha\right|^2\right] > 0 \tag{7.72}$$

then $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} > 0$. This last condition is very easy to satisfy: If the random variables $\omega_1(0), \omega_1(e_1), \omega_1(-e_1), \ldots, \omega_1(e_d), \omega_1(-e_d)$ are independently and identically distributed (i.i.d.), then

$$\mathbb{E}\left[\left|\int_{-\infty}^0 \left\langle w^{(\omega)}, \mathcal{E}(\alpha)\right\rangle_{\mathbb{R}^d} \alpha^2 \mathrm{d}\alpha\right|^2\right] = \mathbb{E}\left[\left|\omega_1(0) - \mathbb{E}\left[\omega_1(0)\right]\right|^2\right] \times \tag{7.73}$$

$$\left(4\left(\int_{-\infty}^0 \langle w, \mathcal{E}(\alpha)\rangle_{\mathbb{R}^d} \alpha^2 \mathrm{d}\alpha\right)^2 + 2\sum_{k=1}^d \left(w_k \int_{-\infty}^0 \left(\mathcal{E}(\alpha)\right)_k \alpha^2 \mathrm{d}\alpha\right)^2\right), \tag{7.74}$$

which is strictly positive for any non-trivial distribution on the measurable space

$$\left([-1,1]^{\mathbb{Z}^d}, \mathfrak{A}_{[-1,1]^{\mathbb{Z}^d}}\right).$$

See Equation (4.1) for the definition of the σ–algebra $\mathfrak{A}_{[-1,1]^{\mathbb{Z}^d}}$.

7.7 Combes-Thomas estimates

For any operator $h \in \mathcal{B}(\mathfrak{h})$ and $\mu \in \mathbb{R}_0^+$, let

$$\mathbf{S}_0(h,\mu) := \sup_{x\in\mathbb{Z}^d} \sum_{y\in\mathbb{Z}^d} \mathrm{e}^{\mu|x-y|} \left|\left\langle \mathfrak{e}_x, h\mathfrak{e}_y\right\rangle_{\mathfrak{h}}\right| \in \mathbb{R}_0^+ \cup \{\infty\}. \tag{7.75}$$

Note that

$$\mathbf{S}_0(h_1h_2,\mu) \leq \mathbf{S}_0(h_1,\mu)\mathbf{S}_0(h_2,\mu), \tag{7.76}$$

for any $h_1, h_2 \in \mathcal{B}(\mathfrak{h})$ and $\mu \in \mathbb{R}_0^+$. In particular, for any $z \in \mathbb{C}$, $h \in \mathcal{B}(\mathfrak{h})$ and $\mu \in \mathbb{R}_0^+$,

$$\mathbf{S}_0(\mathrm{e}^{zh},\mu) \leq \mathrm{e}^{\mathbf{S}_0(zh,\mu)} = \mathrm{e}^{|z|\mathbf{S}_0(h,\mu)} \tag{7.77}$$

and hence,

$$\left|\left\langle \mathfrak{e}_x, \mathrm{e}^{zh}\mathfrak{e}_y\right\rangle_{\mathfrak{h}}\right| \leq \mathrm{e}^{|z|\mathbf{S}_0(h,\mu)}\mathrm{e}^{-\mu|x-y|}.$$

The bound obtained here can be sharpened if $z = it$ is imaginary by using Combes-Thomas estimates, first proven in [36]. To this end, we present a version of this estimate that is adapted to the present setting: Given a self-adjoint operator $h = h^* \in \mathcal{B}(\mathfrak{h})$ whose spectrum is denoted by spec(h), we define the constants

$$\mathbf{S}(h,\mu) := \sup_{x\in\mathbb{Z}^d}\sum_{y\in\mathbb{Z}^d}\left(\mathrm{e}^{\mu|x-y|}-1\right)\left|\left\langle \mathfrak{e}_x, h\mathfrak{e}_y\right\rangle_{\mathfrak{h}}\right| \in \mathbb{R}_0^+\cup\{\infty\}\,, \tag{7.78}$$

for $\mu \in \mathbb{R}_0^+$, and

$$\Delta(h,z) := \inf\{|z-\lambda| : \lambda \in \mathrm{spec}(h)\}\,, \qquad z \in \mathbb{C},$$

as the distance from the point z to the spectrum of h. Since the function $x \mapsto (e^{xr}-1)/x$ is increasing on $\mathbb{R}^+$ for any fixed $r \geq 0$, it follows that

$$\mathbf{S}(h,\mu_1) \leq \frac{\mu_1}{\mu_2}\mathbf{S}(h,\mu_2)\,, \qquad \mu_2 \geq \mu_1 \geq 0. \tag{7.79}$$

The Combes-Thomas estimate we use is the following:

Theorem 7.7.1 (Combes-Thomas)
Let $h = h^* \in \mathcal{B}(\mathfrak{h})$, $\mu \in \mathbb{R}_0^+$ and $z \in \mathbb{C}$. If $\Delta(h,z) > \mathbf{S}(h,\mu)$ then, for all $x,y \in \mathbb{Z}^d$,

$$\left|\left\langle \mathfrak{e}_x, (z-h)^{-1}\mathfrak{e}_y\right\rangle\right| \leq \frac{\mathrm{e}^{-\mu|x-y|}}{\Delta(h,z)-\mathbf{S}(h,\mu)}.$$

Proof: This proposition is a version of the first part of [23, Theorem 10.5] and is proven in the same way. ■

The Combes-Thomas estimate implies the following bound [20, Lemma 3]:

Proposition 7.7.1 (Bound on differences of resolvents)
Let $h = h^* \in \mathcal{B}(\mathfrak{h})$, $\mu \in \mathbb{R}_0^+$ and $\eta \in \mathbb{R}^+$ such that $\mathbf{S}(h,\mu) \leq \eta/2$. Then, for all $x,y \in \mathbb{Z}^d$ and $u \in \mathbb{R}$,

$$\begin{aligned}&\left|\left\langle \mathfrak{e}_x, ((h-u)^2+\eta^2)^{-1}\mathfrak{e}_y\right\rangle_{\mathfrak{h}}\right| \\ &\leq 12\mathrm{e}^{-\mu|x-y|}\left\langle \mathfrak{e}_x, ((h-u)^2+\eta^2)^{-1}\mathfrak{e}_x\right\rangle_{\mathfrak{h}}^{1/2}\left\langle \mathfrak{e}_y, ((h-u)^2+\eta^2)^{-1}\mathfrak{e}_y\right\rangle_{\mathfrak{h}}^{1/2}.\end{aligned}$$

We are now in a position to prove the space decay of propagators:

Corollary 7.7.2 (Space decay of propagators – I)
For any self-adjoint operator $h = h^* \in \mathcal{B}(\mathfrak{h})$, $\eta,\mu \in \mathbb{R}^+$, all $x,y \in \mathbb{Z}^d$ and $t \in \mathbb{R}$,

$$\left|\left\langle \mathfrak{e}_x, \mathrm{e}^{ith}\mathfrak{e}_y\right\rangle_{\mathfrak{h}}\right| \leq 36\mathrm{e}^{\left(|t\eta|-\mu\min\left\{1,\frac{\eta}{2\mathbf{S}(h,\mu)}\right\}|x-y|\right)}.$$

Proof: The proof is a simple adaptation of the one from [20, Theorem 3]: Fix all parameters of the lemma and observe that Proposition 7.7.1 combined with Inequality (7.79) yields

$$\left|\left\langle \mathfrak{e}_x, ((h-u)^2+\eta^2)^{-1}\mathfrak{e}_y\right\rangle_{\mathfrak{h}}\right| \tag{7.80}$$

$$\leq 12\mathrm{e}^{-\frac{\mu\eta}{2\mathbf{S}(h,\mu)}|x-y|}\left\langle \mathfrak{e}_x, ((h-u)^2+\eta^2)^{-1}\mathfrak{e}_x\right\rangle_{\mathfrak{h}}^{1/2}\left\langle \mathfrak{e}_y, ((h-u)^2+\eta^2)^{-1}\mathfrak{e}_y\right\rangle_{\mathfrak{h}}^{1/2} \tag{7.81}$$

for $x, y \in \mathbb{Z}^d$, $u \in \mathbb{R}$ and $\eta \in \mathbb{R}^+$. On the other hand, at fixed $\eta \in \mathbb{R}^+$, the function defined by $G(z) := \mathrm{e}^{itz}$ on the stripe

$$\mathbb{R} + i\eta\,[-1,1] \subset \mathbb{C}$$

is analytic and uniformly bounded by $\mathrm{e}^{|t\eta|}$. Using Cauchy's integral formula and some translation by $\pm i\eta$, we write the function G as

$$G(E) = \frac{1}{2\pi i}\int_{R_\eta}\frac{\mathrm{e}^{itu}}{u-E}\mathrm{d}u. \tag{7.82}$$

where R_η is the rectangle defined by $(\pm R \pm i\eta)$. Furthermore,

$$\begin{aligned}\left|\int_{-\eta}^{\eta}\frac{G(R+iu)}{R+iu-E}i\mathrm{d}u\right| &\leq \int_{-\eta}^{\eta}\left|\frac{\mathrm{e}^{it(R+iu)}}{R+iu-E}\right|\mathrm{d}u\\ &= \int_{-\eta}^{\eta}\left|\frac{\mathrm{e}^{-tu}}{R+iu-E}\right|\mathrm{d}u\\ &= \int_{-\eta}^{\eta}\left|\frac{\mathrm{e}^{-tu}}{\sqrt{(R-E)^2+u^2}}\right|\mathrm{d}u\\ &\leq \frac{1}{|R-E|}\int_{-\eta}^{\eta}\mathrm{e}^{-tu}\mathrm{d}u\end{aligned}$$

It remains true for

$$\left|\int_{\eta}^{-\eta}\frac{G(-R+iu)}{-R+iu-E}i\mathrm{d}u\right|$$

By taking $R \to \infty$, the remaining term is

$$\begin{aligned}G(E) &= \frac{1}{2\pi i}\int_{\mathbb{R}}\left(\frac{G(u-i\eta)}{u-i\eta-E} - \frac{G(u+i\eta)}{u+i\eta-E}\right)\mathrm{d}u\\ &= \frac{\eta}{\pi}\int_{\mathbb{R}}\frac{G(u-i\eta)+G(u+i\eta)}{(E-u)^2+\eta^2}\mathrm{d}u - \frac{2\eta}{\pi}\int_{\mathbb{R}}\frac{G(u)}{(E-u)^2+4\eta^2}\mathrm{d}u\end{aligned}$$

for all $E \in \mathbb{R}$ and $\eta \in \mathbb{R}^+$. By spectral calculus, together with (7.80) and the Cauchy-Schwarz inequality, the assertion follows for e^{ith}. ■

Corollary 7.7.3 (Space decay of propagators – II)
For any self-adjoint operators $h_1, h_2 \in \mathcal{B}(\mathfrak{h})$ and all $x, y \in \mathbb{Z}^d$,

$$\left| \left\langle \mathfrak{e}_x, \frac{1}{1 + \mathrm{e}^{h_2}\mathrm{e}^{h_1}\mathrm{e}^{h_2}} \mathfrak{e}_y \right\rangle_{\mathfrak{h}} \right| \leq 2 \inf_{\mu \in \mathbb{R}_0^+} \mathrm{e}^{\left(-\frac{\mu}{2}\mathrm{e}^{-\mathbf{S}_0(h_1,\mu)-2\mathbf{S}_0(h_2,\mu)}|x-y|\right)}.$$

Proof: By (7.75)-(7.78), note that, for any $\mu \in \mathbb{R}_0^+$,

$$\mathbf{S}(\mathrm{e}^{h_2}\mathrm{e}^{h_1}\mathrm{e}^{h_2}, \mu) \leq \mathbf{S}_0(\mathrm{e}^{h_2}\mathrm{e}^{h_1}\mathrm{e}^{h_2}, \mu) \leq \mathrm{e}^{\mathbf{S}_0(h_1,\mu)+2\mathbf{S}_0(h_2,\mu)}.$$

Fix $\mu \in \mathbb{R}_0^+$ and define

$$\mu_1 := \frac{\mu}{2}\mathrm{e}^{-\mathbf{S}_0(h_1,\mu)-2\mathbf{S}_0(h_2,\mu)}.$$

By (7.79), $\mathbf{S}(\mathrm{e}^{h_2}\mathrm{e}^{h_1}\mathrm{e}^{h_2}, \mu_1) < 1/2$. Meanwhile, by using Theorem 7.7.1 with $h = \mathrm{e}^{h_2}\mathrm{e}^{h_1}\mathrm{e}^{h_2} \geq 0$,

$$\left| \left\langle \mathfrak{e}_x, \frac{1}{1 + \mathrm{e}^{h_2}\mathrm{e}^{h_1}\mathrm{e}^{h_2}} \mathfrak{e}_y \right\rangle_{\mathfrak{h}} \right| \leq 2\mathrm{e}^{-\mu_1|x-y|}.$$

■

7.8 Electromagnetic Energy produced in a Ring

Within this section, we give some estimates and results in order to understand the heat transport properties for free fermions in a disordered media. This is a very preliminary step towards the derivation of the Heat equation.

Let $\mathcal{A} \in C_0^\infty(\mathbb{R}; \mathbb{R}^d)$ and set $\mathcal{E}(t) \doteq -\partial_t \mathcal{A}(t)$ for all $t \in \mathbb{R}$. Then, in all this section, $\mathbf{A}$ is defined to be the vector potential such that the electric field is given by $\mathcal{E}(t) \in C_0^\infty(\mathbb{R}; \mathbb{R}^d)$ at time $t \in \mathbb{R}$, for all $x \in [-1, 1]^d$, and $(0, 0, \ldots, 0)$ for $t \in \mathbb{R}$ and $x \notin [-1, 1]^d$. It yields a rescaled vector potential $\eta \mathbf{A}_\ell$, for $\ell \in \mathbb{R}^+$ and $\eta \in \mathbb{R}_0^+$. See (4.31). The electromagnetic potential perturbs the free dynamics. This is given, in the algebraic formulation, by a bounded pertubation of the derivation generated the free systems, defined by the commutator $[W_t^{(\eta \mathbf{A}_\ell)}, \cdot]$ with

$$W_t^{(\eta \mathbf{A}_\ell)} := \sum_{x,y \in \mathbb{Z}^d} \langle \mathfrak{e}_x, \Theta_{t,\ell} \mathfrak{e}_y \rangle_{\mathfrak{h}} a^*(\mathfrak{e}_x) a(\mathfrak{e}_y) \tag{7.83}$$

for any $t \in \mathbb{R}$ and $\ell \in \mathbb{R}^+$. Here, for any $t \in \mathbb{R}$ and $\ell \in \mathbb{R}^+$,

$$\Theta_{t,\ell} := \Delta_{\omega,\vartheta}^{(\eta \mathbf{A}_\ell)} - \Delta_{\omega,\vartheta} = \mathcal{O}(\eta). \tag{7.84}$$

the sef-adjoint operator $\Delta_{\omega,\vartheta}^{(\eta \mathbf{A}_\ell)}$ being taken at time t. See Equation (4.23).

As explained in Section 4.3.3, in order to understand heat transport properties, one can study the energy propagation in a finite ring contained in $\mathbb{Z}^d$. Here, we refer to the ring

$\mathcal{R}_\ell$ that has been defined for $\ell \in \mathbb{R}^+$ by (4.37). The explicit form of the ring is not used here and, for any $\ell \in \mathbb{R}^+$, we denote by $\mathcal{R}_\ell$ any finite region such that $\mathcal{R}_\ell \cap \Lambda_\ell = \emptyset$ and such that

$$|\mathcal{R}_\ell|^{-1} |\partial \mathcal{R}_\ell| = o(1), \qquad \ell \in \mathbb{R}^+, \tag{7.85}$$

where $|\partial \mathcal{R}_\ell|$ denote the volume of the surface terms of $\mathcal{R}_\ell$. Since $\mathcal{R}_\ell \cap \Lambda_\ell = \emptyset$, recall also that the energy density observable within the region $\mathcal{R}_\ell$ is equal to

$$\mathfrak{E}_{\mathcal{R}_\ell}^{(\omega)} := \frac{1}{|\mathcal{R}_\ell|} \sum_{x,y \in \mathcal{R}_\ell} \langle \mathfrak{e}_x, h^{(\omega)} \mathfrak{e}_y \rangle_{\mathfrak{h}} a^*(\mathfrak{e}_x) a(\mathfrak{e}_y), \quad \ell \in \mathbb{R}^+. \tag{7.86}$$

Under the external electromagnetic potential applied in the finite cubic box Λ_ℓ of the lattice for $\ell \in \mathbb{R}^+$, one can observe the heat transport within the region $\mathcal{R}_\ell$ satisfying $\mathcal{R}_\ell \cap \Lambda_\ell = \emptyset$. The time evolution with respect to the non-autonomous dynamics yields an energy density increment observable defined by (4.38), that is, for any $\ell \in \mathbb{R}^+$ and $\eta \in \mathbb{R}$,

$$\epsilon_{\mathcal{R}_\ell}^{(\omega)}(\eta, t) := \tau_{t,0}^{(\omega, \eta \mathbf{A}_\ell)} \left(\mathfrak{E}_{\mathcal{R}_\ell}^{(\omega)} \right) - \tau_t^{(\omega)} \left(\mathfrak{E}_{\mathcal{R}_\ell}^{(\omega)} \right).$$

In order to study this time evolution of the energy, we first recall the definition of multi-commutators. Multi-commutators are straightforward extensions of the concept of commutators

$$[B_1, B_2] := B_1 B_2 - B_2 B_1 , \qquad B_1, B_2 \in \mathcal{U} .$$

They are defined as follows:

Definition 7.8.1 (Multi-commutators)
By induction, for all integers $k > 1$,

$$[B_1, B_2, \ldots, B_{k+1}]^{(k+1)} := [B_1, [B_2, \ldots, B_{k+1}]^{(k)}] , \qquad B_1, \ldots, B_{k+1} \in \mathcal{U}$$

where

$$[B_1, B_2]^{(2)} := [B_1, B_2] , \qquad B_1, B_2 \in \mathcal{U} .$$

The last definition is important since multi-commutators appear in (partial) Dyson-Phillips series associated with increment observables. Indeed, for any $B \in \mathcal{U}$, from (4.25), similar to [31, Theorem 5.7], it is easy to check that

$$\begin{aligned}
\tau_{t,s}^{(\omega,\mathbf{A})}(B) - \tau_t^{(\omega)}(B) = {} & i \int_0^t \mathrm{d}s_1 \left[\tau_{s_1}^{(\omega)}(W_{s_1}^{(\mathbf{A})}), \tau_t^{(\omega)}(B) \right]^{(2)} \\
& + i^2 \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \left(\left[\tau_{s_2}^{(\omega)} \left(W_{s_2}^{(\mathbf{A})} \right), \tau_{s_1}^{(\omega)} \left(W_{s_1}^{(\mathbf{A})} \right), \tau_t^{(\omega)}(B)) \right]^{(3)} \right) \\
& + i^3 \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \int_0^{s_2} \mathrm{d}s_3 \tau_{s_3,0}^{(\omega,\mathbf{A})} \left(\left[W_{s_3}^{(\mathbf{A})}, \tau_{s_2 - s_3}^{(\omega)} \left(W_{s_2}^{(\mathbf{A})} \right), \tau_{s_1 - s_3}^{(\omega)} \left(W_{s_1}^{(\mathbf{A})} \right), \tau_{t - s_3}^{(\omega)}(B)) \right]^{(4)} \right).
\end{aligned}$$

By applying the last equality to (7.86) and (4.38), one obtains that

$$\epsilon_{\mathcal{R}_\ell}^{(\omega)}(\eta) = i\int_0^t \mathrm{d}s_1 \left[\tau_{s_1}^{(\omega)}(W_{s_1}^{\eta\mathbf{A}_\ell}), \tau_t^{(\omega)}(\mathfrak{E}_{\mathcal{R}_\ell}^{(\omega)})\right]^{(2)} \tag{7.87}$$

$$+ i^2\int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \left(\left[\tau_{s_2}^{(\omega)}\left(W_{s_2}^{(\eta\mathbf{A}_\ell)}\right), \tau_{s_1}^{(\omega)}\left(W_{s_1}^{(\eta\mathbf{A}_\ell)}\right), \tau_t^{(\omega)}(\mathfrak{E}_{\mathcal{R}_\ell}^{(\omega)}))\right]^{(3)}\right) \tag{7.88}$$

$$+ \mathcal{O}\left(\eta^3\right). \tag{7.89}$$

The fact that the remaining term of order $\mathcal{O}(\eta^3)$ is clear since

$$W_{s_2}^{(\eta\mathbf{A}_\ell)} = \mathcal{O}(\eta\,|\Lambda_\ell|), \qquad \ell \in \mathbb{R}^+.$$

What is *absolutely not* trivial is the fact that this order term can be bounded *uniformly* for all $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\ell \in \mathbb{R}^+$, $t \in \mathbb{R}_0^+$ and ϑ, t in compact sets of $\mathbb{R}_0^+$ and $\mathbb{R}$, respectively. This is an important and pivotal property since we are interested in knowing the energy density increment in the limit $\ell \to \infty$. This property is a consequence of Taylor's theorem for increments [31, Theorem 4.15], which is in fact a consequence of the Lieb Robinson bound for multi-commutators (see, e.g., [31, Corollary 4.12]).

We are now in a position to compute explicitly the first terms in the expansion (7.89) of the energy density increment.

Lemma 7.8.2 (Linear energy term)
For all $t, s \in \mathbb{R}$, $\omega \in \Omega$, $\lambda, \vartheta, \eta \in \mathbb{R}_0^+$ and $\ell \in \mathbb{R}^+$,

$$i\int_0^t \mathrm{d}s_1 \varrho^{(\omega)}\left(\left[\tau_{s_1}^{(\omega)}(W_{s_1}^{(\mathbf{A})}), \tau_t^{(\omega)}(\mathfrak{E}_{\mathcal{R}_\ell}^{(\omega,\lambda)})\right]^{(2)}\right) = \int_0^t \mathrm{d}s_1 \frac{1}{|\mathcal{R}_\ell|}\mathrm{Tr}_{\mathfrak{h}}\left(\mathfrak{D}_{\mathcal{R}_\ell,\omega,\beta}\mathrm{e}^{i(s_1-t)h^{(\omega)}}\Theta_{s_1,\ell}\mathrm{e}^{i(t-s_1)h^{(\omega)}}\right)$$

with $\mathrm{Tr}_{\mathfrak{h}}$ being the trace on $\mathfrak{h} := \ell^2(\mathbb{Z}^d)$, $P_{\mathcal{R}_\ell}$ the orthogonal projection defined on $\mathfrak{h}$ by (4.9) for $\Lambda = \mathcal{R}_\ell$ and

$$\mathfrak{D}_{\mathcal{R}_\ell,\omega,\beta} := i\left[P_{\mathcal{R}_\ell}h^{(\omega)}P_{\mathcal{R}_\ell}, (1+\mathrm{e}^{\beta h^{(\omega)}})^{-1}\right]. \tag{7.90}$$

Proof: Fix all parameters of the lemma. By (7.83) and (7.86), for any $\ell \in \mathbb{R}^+$ and $\alpha, s_1 \in \mathbb{R}$ ($\alpha = s_1 - t$),

$$\mathbf{X}_{\alpha,\ell} := i[\tau_\alpha^{(\omega)}(W_{s_1}^{\eta\mathbf{A}_\ell}), \mathfrak{E}_{\mathcal{R}_\ell}^{(\omega,\lambda)}] = \frac{1}{|\mathcal{R}_\ell|}\sum_{x,y\in\mathbb{Z}^d}\sum_{z,w\in\mathcal{R}_\ell}\langle \mathfrak{e}_x, \Theta_{s_1,\ell}\mathfrak{e}_y\rangle_{\mathfrak{h}}\langle \mathfrak{e}_z, h^{(\omega)}\mathfrak{e}_w\rangle_{\mathfrak{h}} \tag{7.91}$$

$$\times\, i\left[\tau_\alpha^{(\omega)}(a^*(\mathfrak{e}_x))\tau_\alpha^{(\omega)}(a(\mathfrak{e}_y)), a^*(\mathfrak{e}_z)a(\mathfrak{e}_w)\right]. \tag{7.92}$$

Since, for any $x, y, z, w \in \mathbb{Z}^d$,

$$\begin{aligned}&\left[\tau_\alpha^{(\omega)}(a^*(\mathfrak{e}_x))\,\tau_\alpha^{(\omega)}\left(a(\mathfrak{e}_y)\right), a^*(\mathfrak{e}_z)a(\mathfrak{e}_w)\right]\\ =\;& \left\langle \mathrm{e}^{i\alpha h^{(\omega)}}\mathfrak{e}_y, \mathfrak{e}_z\right\rangle_{\mathfrak{h}}\tau_\alpha^{(\omega)}(a^*(\mathfrak{e}_x))\,a(\mathfrak{e}_w) - \left\langle \mathfrak{e}_w, \mathrm{e}^{i\alpha h^{(\omega)}}\mathfrak{e}_x\right\rangle_{\mathfrak{h}} a^*(\mathfrak{e}_z)\tau_\alpha^{(\omega)}\left(a(\mathfrak{e}_y)\right)\end{aligned}$$

we arrive at

$$\mathbf{X}_{\alpha,\ell} = \frac{2}{|\mathcal{R}_\ell|} \sum_{x,y\in\mathbb{Z}^d} \sum_{z,w\in\mathcal{R}_\ell} \mathfrak{Im}\left(\langle \mathfrak{e}_y, \Theta_{s_1,\ell}\mathfrak{e}_x\rangle_{\mathfrak{h}} \langle \mathfrak{e}_w, h^{(\omega)}\mathfrak{e}_z\rangle_{\mathfrak{h}} \left\langle \mathfrak{e}_z, \mathrm{e}^{i\alpha h^{(\omega)}}\mathfrak{e}_y\right\rangle_{\mathfrak{h}} a^*(\mathfrak{e}_w)\tau_\alpha^{(\omega)}(a(\mathfrak{e}_x))\right) \tag{7.93}$$

for any $\ell \in \mathbb{R}^+$ and $\alpha \in \mathbb{R}$. Furthermore, by (4.18) and (4.20), observe that, for any $w, x \in \mathbb{Z}^d$ and $\alpha_1, \alpha_2 \in \mathbb{R}$,

$$\varrho^{(\omega)}\left(\tau_{\alpha_2}^{(\omega)}(a^*(\mathfrak{e}_w))\,\tau_{\alpha_1}^{(\omega)}(a(\mathfrak{e}_x))\right) = \left\langle \mathfrak{e}_x, \frac{\mathrm{e}^{i(\alpha_2-\alpha_1)h^{(\omega)}}}{1+\mathrm{e}^{\beta h^{(\omega)}}}\mathfrak{e}_w\right\rangle_{\mathfrak{h}}. \tag{7.94}$$

It follows that

$$\begin{aligned}&\varrho^{(\omega)}(\mathbf{X}_{\alpha,\ell})\\ &= \frac{2}{|\mathcal{R}_\ell|} \sum_{x,y\in\mathbb{Z}^d} \sum_{z,w\in\mathcal{R}_\ell} \mathfrak{Im}\left(\langle \mathfrak{e}_y, \Theta_{s_1,\ell}\mathfrak{e}_x\rangle_{\mathfrak{h}} \langle \mathfrak{e}_w, h^{(\omega)}\mathfrak{e}_z\rangle_{\mathfrak{h}} \left\langle \mathfrak{e}_z, \mathrm{e}^{i\alpha h^{(\omega)}}\mathfrak{e}_y\right\rangle_{\mathfrak{h}} \left\langle \mathfrak{e}_x, \frac{\mathrm{e}^{-i\alpha h^{(\omega)}}}{1+\mathrm{e}^{\beta h^{(\omega)}}}\mathfrak{e}_w\right\rangle_{\mathfrak{h}}\right)\end{aligned}$$

which, by elementary manipulations using the cyclicity of the trace $\mathrm{Tr}_{\mathfrak{h}}$ on $\mathfrak{h} := \ell^2(\mathbb{Z}^d)$, can be rewritten as

$$\varrho^{(\omega)}(\mathbf{X}_{\alpha,\ell}) \tag{7.95}$$

$$= \frac{2}{|\mathcal{R}_\ell|} \sum_{y\in\mathbb{Z}^d} \mathfrak{Im}\left\langle \mathfrak{e}_y, \Theta_{s_1,\ell}\frac{\mathrm{e}^{-i\alpha h^{(\omega)}}}{1+\mathrm{e}^{\beta h^{(\omega)}}} P_{\mathcal{R}_\ell} h^{(\omega)} P_{\mathcal{R}_\ell} \mathrm{e}^{i\alpha h^{(\omega)}}\mathfrak{e}_y\right\rangle_{\mathfrak{h}} \tag{7.96}$$

$$= \frac{1}{|\mathcal{R}_\ell|}\mathrm{Tr}_{\mathfrak{h}}\left(\mathfrak{D}_{\mathcal{R}_\ell,\omega,\beta}\mathrm{e}^{i\alpha h^{(\omega)}}\Theta_{s_1,\ell}\mathrm{e}^{-i\alpha h^{(\omega)}}\right) \tag{7.97}$$

for any $\ell \in \mathbb{R}^+$ and $\alpha \in \mathbb{R}$, with $P_{\mathcal{R}_\ell}$ being the orthogonal projection defined on $\mathfrak{h}$ by (4.9) for $\Lambda = \mathcal{R}_\ell$ and $\mathfrak{D}_{\mathcal{R}_\ell,\omega,\beta}$ defined by (7.90). ■

Lemma 7.8.3
For all $t, s \in \mathbb{R}$,

$$\lim_{\ell\to\infty}\left(i\int_0^t \mathrm{d}s_1 \varrho^{(\omega)}\left(\left[\tau_{s_1}^{(\omega)}(W_{s_1}^{(\mathbf{A})}), \tau_t^{(\omega)}(\mathfrak{E}_{\mathcal{R}_\ell}^{(\omega,\lambda)})\right]^{(2)}\right)\right) = 0$$

uniformly with respect to $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\ell \in \mathbb{R}^+$, $t \in \mathbb{R}_0^+$ and ϑ, t in compact sets of $\mathbb{R}_0^+$ and $\mathbb{R}$, respectively.

Proof: By (7.90), note that

$$\mathfrak{D}_{\mathcal{R}_\ell,\omega,\beta} = i\left(\left[P_{\mathcal{R}_\ell}, (1+\mathrm{e}^{\beta h^{(\omega)}})^{-1}\right] h^{(\omega)} P_{\mathcal{R}_\ell} + P_{\mathcal{R}_\ell} h^{(\omega)}\left[P_{\mathcal{R}_\ell}, (1+\mathrm{e}^{\beta h^{(\omega)}})^{-1}\right]\right)$$

while

$$\left[P_{\mathcal{R}_\ell}, (1+\mathrm{e}^{\beta h^{(\omega)}})^{-1}\right] = (1+\mathrm{e}^{\beta h^{(\omega)}})^{-1}\left[\mathrm{e}^{\beta h^{(\omega)}}, P_{\mathcal{R}_\ell}\right](1+\mathrm{e}^{\beta h^{(\omega)}})^{-1}.$$

Since $h^{(\omega)}$ bounded, the series for $\mathrm{e}^{\beta h^{(\omega)}}$ absolutely converges and

$$\left[P_{\mathcal{R}_\ell},(1+\mathrm{e}^{\beta h^{(\omega)}})^{-1}\right]=(1+\mathrm{e}^{\beta h^{(\omega)}})^{-1}\sum_{k\in\mathbb{N}}\frac{\beta^k}{k!}\left[\left(h^{(\omega)}\right)^k,P_{\mathcal{R}_\ell}\right](1+\mathrm{e}^{\beta h^{(\omega)}})^{-1}$$

with

$$\begin{aligned}&\sum_{k\in\mathbb{N}}\frac{\beta^k}{k!}\left[\left(h^{(\omega)}\right)^k,P_{\mathcal{R}_\ell}\right]\\ &=\beta\left[h^{(\omega)},P_{\mathcal{R}_\ell}\right]+\frac{\beta^2}{2!}\left(h^{(\omega)}\left[h^{(\omega)},P_{\mathcal{R}_\ell}\right]+\left[h^{(\omega)},P_{\mathcal{R}_\ell}\right]h^{(\omega)}\right)\\ &\quad+\frac{\beta^3}{3!}\left(\left(h^{(\omega)}\right)^2\left[h^{(\omega)},P_{\mathcal{R}_\ell}\right]+h^{(\omega)}\left[h^{(\omega)},P_{\mathcal{R}_\ell}\right]h^{(\omega)}+\left[h^{(\omega)},P_{\mathcal{R}_\ell}\right]\left(h^{(\omega)}\right)^2\right)+\cdots\\ &\quad+\frac{\beta^k}{k!}\left(\left(h^{(\omega)}\right)^{k-1}\left[h^{(\omega)},P_{\mathcal{R}_\ell}\right]+\left(h^{(\omega)}\right)^{k-2}\left[h^{(\omega)},P_{\mathcal{R}_\ell}\right]h^{(\omega)}+\cdots+\left[h^{(\omega)},P_{\mathcal{R}_\ell}\right]\left(h^{(\omega)}\right)^{k-1}\right)\\ &\quad+\cdots\end{aligned}$$

The commutator

$$\left[h^{(\omega)},P_{\mathcal{R}_\ell}\right]=[\Delta_{\omega,\vartheta},P_{\mathcal{R}_\ell}]$$

can be explicitly computed and clearly involved $o\left(|\mathcal{R}_\ell|\right)$ terms, only, by (7.85). In fact, it involves a surface term with respect to $\mathcal{R}_\ell$ and this commutator has the form

$$\left[h^{(\omega)},P_{\mathcal{R}_\ell}\right]=\sum_{w\in\mathcal{Z}_\ell}\sum_{z\in\mathfrak{L},\ |z|=1}C_{w,z}^{(\omega,\vartheta)}P_{\{w\}}$$

for some finite set $\mathcal{Z}_\ell\subseteq\mathbb{Z}^d$ of volume $|\mathcal{Z}_\ell|=o\left(|\mathcal{R}_\ell|\right)$ as $\ell\to\infty$,

$$\left\{C_{w,z}^{(\omega,\vartheta)}\right\}_{w,z\in\mathbb{Z}^d}\subset\mathbb{C}$$

being a set of complex numbers such that

$$\sup_{\vartheta\in[0,\vartheta_0]}\ \sup_{\omega\in\Omega}\ \sup_{w,z\in\mathbb{Z}^d}C_{w,z}^{(\omega,\vartheta)}<\infty\ .$$

Note from Lemma 7.8.2 that

$$\varrho^{(\omega)}\left(\mathbf{X}_{\alpha,\ell}\right)=\frac{1}{|\mathcal{R}_\ell|}\sum_{x,y\in\mathbb{Z}^d}\left\langle\mathfrak{e}_y,\mathfrak{D}_{\mathcal{R}_\ell,\omega,\beta}\mathfrak{e}_x\right\rangle_{\mathfrak{h}}\left\langle\mathfrak{e}_x,\mathrm{e}^{i\alpha h^{(\omega)}}\Theta_{s_1,\ell}\mathrm{e}^{-i\alpha h^{(\omega)}}\mathfrak{e}_y\right\rangle_{\mathfrak{h}}\tag{7.98}$$

for any $\ell\in\mathbb{R}^+$ and $\alpha\in\mathbb{R}$. By the Combes-Thomas estimates, in particular, (4.13) and Corollary 7.7.3, (7.98) can be written as a sum of the form

$$\frac{1}{|\mathcal{R}_\ell|}\sum_{w\in\mathcal{Z}_\ell}\sum_{x,y\in\mathbb{Z}^d}\mathbf{Y}_{\ell,\alpha}^{(\omega)}\left(w,x,y\right)$$

for which the sum over $x,y\in\mathbb{Z}^d$ is absolutly convergent with respect to $\omega\in\Omega$, $\lambda\in\mathbb{R}_0^+$, $\ell\in\mathbb{R}^+$, $t\in\mathbb{R}_0^+$, $w\in\mathbb{Z}^d$, and ϑ,α in compact sets of $\mathbb{R}_0^+$ and $\mathbb{R}$, respectively. Because $|\mathcal{Z}_\ell| = o(|\mathcal{R}_\ell|)$ as $\ell\to\infty$, by (7.85), we thus obtain that

$$\lim_{\ell\to\infty}\mathbf{X}_{\alpha,\ell}=0$$

for any $\alpha\in\mathbb{R}$, uniformly with respect to $\omega\in\Omega$, $\lambda\in\mathbb{R}_0^+$, $\ell\in\mathbb{R}^+$, $t\in\mathbb{R}_0^+$ and ϑ,α in compact sets of $\mathbb{R}_0^+$ and $\mathbb{R}$, respectively. The assertion then follows. ∎

Note that a similar results as Lemmata 7.8.2-7.8.3 can be obtained for the time derivative

$$\partial_t\left(i\int_0^t \mathrm{d}s_1\varrho^{(\omega)}\left(\left[\tau_{s_1}^{(\omega)}(W_{s_1}^{(\mathbf{A})}),\tau_t^{(\omega)}(B)\right]^{(2)}\right)\right).$$

We refrain from doing this to focus our study on the main term of $\epsilon_{\mathcal{R}_\ell}^{(\omega)}(\eta)$ as $\ell\to\infty$, which, by Lemma 7.8.2 and (7.89), is of order $\mathcal{O}(\eta^2)$. In particular, the behavior of the density energy increment at thermodynamic limit (large ℓ), with respect to $\eta\in\mathbb{R}^+$, relies on the asymptotic behavior of

$$\mathbf{Z}_{\ell,t}^{(\omega,\mathbf{A})} := -\eta^{-2}\int_0^t \mathrm{d}s_1\int_0^{s_1}\mathrm{d}s_2\left(\left[\tau_{s_2}^{(\omega)}\left(W_{s_2}^{(\eta\mathbf{A}_\ell)}\right),\tau_{s_1}^{(\omega)}\left(W_{s_1}^{(\eta\mathbf{A}_\ell)}\right),\tau_t^{(\omega)}(\mathfrak{E}_{\mathcal{R}_\ell}^{(\omega)}))\right]^{(3)}\right),$$

which is of order

$$\mathbf{Z}_{\ell,t}^{(\omega,\mathbf{A})} = \mathcal{O}(1),$$

uniformly with respect to $\omega\in\Omega$, $\lambda,\ell\in\mathbb{R}_0^+$ and t in compact sets, by Taylor's theorem for increments [31, Theorem 4.15] (in fact the Lieb Robinson bound for multi-commutators, see, e.g., [31, Corollary 4.12]). We give here an explicit expression of $\varrho^{(\omega)}(\mathbf{Z}_{\ell,t}^{(\omega,\mathbf{A})})$ in terms of the one-particle Hilbert space $\mathfrak{h}$:

Lemma 7.8.4 (Quadratic energy term)
For all $t,s\in\mathbb{R}$, $\omega\in\Omega$, $\lambda,\vartheta,\eta\in\mathbb{R}_0^+$ and $\ell\in\mathbb{R}^+$,

$$\begin{aligned}\varrho^{(\omega)}\left(\mathbf{Z}_{\ell,t}^{(\omega,\mathbf{A})}\right) = & -\eta^{-2}\int_0^t\mathrm{d}s_1\int_0^{s_1}\mathrm{d}s_2\frac{i}{|\mathcal{R}_\ell|}\mathrm{Tr}_{\mathfrak{h}}\left(P_{\mathcal{R}_\ell}h^{(\omega)}P_{\mathcal{R}_\ell}\mathrm{e}^{i(s_2-t)h^{(\omega)}}\mathfrak{Q}_{s_2,\ell}^{(\omega)}\mathrm{e}^{i(s_1-s_2)h^{(\omega)}}\Theta_{s_1,\ell}\mathrm{e}^{i(t-s_1)h^{(\omega)}}\right)\\ & -\eta^{-2}\int_0^t\mathrm{d}s_1\int_0^{s_1}\mathrm{d}s_2\frac{i}{|\mathcal{R}_\ell|}\mathrm{Tr}_{\mathfrak{h}}\left(\Theta_{s_1,\ell}\mathrm{e}^{i(s_2-t)h^{(\omega)}}\mathfrak{Q}_{s_2,\ell}^{(\omega)}\mathrm{e}^{i(s_1-s_2)h^{(\omega)}}P_{\mathcal{R}_\ell}h^{(\omega)}P_{\mathcal{R}_\ell}\mathrm{e}^{i(s_1-t)h^{(\omega)}}\right)\end{aligned}$$

with $\mathrm{Tr}_{\mathfrak{h}}$ being the trace on $\mathfrak{h}:=\ell^2(\mathbb{Z}^d)$, $P_{\mathcal{R}_\ell}$ the orthogonal projection defined on $\mathfrak{h}$ by (4.9) for $\Lambda=\mathcal{R}_\ell$ and

$$\mathfrak{Q}_{s_2,\ell}^{(\omega)} := \left[\left(1+\mathrm{e}^{\beta h^{(\omega)}}\right)^{-1},\Theta_{s_2,\ell}\right].$$

Proof: Fix all parameters of the lemma. Similar to (7.91) and (7.93), for any $s_1,s_2,t\in\mathbb{R}$, the element

$$\mathbf{K} := \left[\tau_{s_2}^{(\omega)}\left(W_{s_2}^{(\eta\mathbf{A}_\ell)}\right),\tau_{s_1}^{(\omega)}\left(W_{s_1}^{(\eta\mathbf{A}_\ell)}\right),\tau_t^{(\omega)}(\mathfrak{E}_{\mathcal{R}_\ell}^{(\omega)}))\right]^{(3)}$$

is equal to

$$\mathbf{K} = \frac{i}{|\mathcal{R}_\ell|}\sum_{x,y,u,v\in\mathbb{Z}^d}\sum_{z,w\in\mathcal{R}_\ell}\langle \mathrm{e}_u,\Theta_{s_2,\ell}\mathrm{e}_v\rangle_{\mathfrak{h}}\langle \mathrm{e}_x,\Theta_{s_1,\ell}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_z,h^{(\omega)}\mathrm{e}_w\rangle_{\mathfrak{h}}\left\langle \mathrm{e}^{i(s_1-t)h^{(\omega)}}\mathrm{e}_y,\mathrm{e}_z\right\rangle_{\mathfrak{h}}$$
$$\times\left[\tau_{s_2}^{(\omega)}\left(a^*(\mathrm{e}_u)\right)\tau_{s_2}^{(\omega)}\left(a(\mathrm{e}_v)\right),\tau_{s_1}^{(\omega)}\left(a^*(\mathrm{e}_x)\right)\tau_{t}^{(\omega)}\left(a(\mathrm{e}_w)\right)\right]$$
$$-\frac{i}{|\mathcal{R}_\ell|}\sum_{x,y,u,v\in\mathbb{Z}^d}\sum_{z,w\in\mathcal{R}_\ell}\langle \mathrm{e}_u,\Theta_{s_2,\ell}\mathrm{e}_v\rangle_{\mathfrak{h}}\langle \mathrm{e}_y,\Theta_{s_1,\ell}\mathrm{e}_x\rangle_{\mathfrak{h}}\langle \mathrm{e}_w,h^{(\omega)}\mathrm{e}_z\rangle_{\mathfrak{h}}\left\langle \mathrm{e}_z,\mathrm{e}^{i(s_1-t)h^{(\omega)}}\mathrm{e}_y\right\rangle_{\mathfrak{h}}$$
$$\times\left[\tau_{s_2}^{(\omega)}\left(a^*(\mathrm{e}_u)\right)\tau_{s_2}^{(\omega)}\left(a(\mathrm{e}_v)\right),\tau_{t}^{(\omega)}\left(a^*(\mathrm{e}_w)\right)\tau_{s_1}^{(\omega)}\left(a(\mathrm{e}_x)\right)\right]$$

where $\Theta_{\alpha,\ell}$ is defined by (7.84). By (3.12) and (4.18), for any $u,v,x,w\in\mathbb{Z}^d$,

$$\begin{aligned}&\left[\tau_{s_2}^{(\omega)}\left(a^*(\mathrm{e}_u)a(\mathrm{e}_v)\right),\tau_{s_1}^{(\omega)}\left(a^*(\mathrm{e}_x)\right)\tau_{t}^{(\omega)}\left(a(\mathrm{e}_w)\right)\right]\\&=\langle \mathrm{e}^{is_2h^{(\omega)}}\mathrm{e}_v,\mathrm{e}^{is_1h^{(\omega)}}\mathrm{e}_x\rangle_{\mathfrak{h}}\tau_{s_2}^{(\omega)}\left(a^*(\mathrm{e}_u)\right)\tau_{t}^{(\omega)}\left(a(\mathrm{e}_w)\right)\\&\quad-\langle \mathrm{e}^{ith^{(\omega)}}\mathrm{e}_w,\mathrm{e}^{is_2h^{(\omega)}}\mathrm{e}_u\rangle_{\mathfrak{h}}\tau_{s_1}^{(\omega)}\left(a^*(\mathrm{e}_x)\right)\tau_{s_2}^{(\omega)}\left(a(\mathrm{e}_v)\right).\end{aligned}$$

Using this together with (7.94), we arrive at

$$\varrho^{(\omega)}(\mathbf{K}) = \frac{i}{|\mathcal{R}_\ell|}\sum_{x,y,u,v\in\mathbb{Z}^d}\sum_{z,w\in\mathcal{R}_\ell}\langle \mathrm{e}_u,\Theta_{s_2,\ell}\mathrm{e}_v\rangle_{\mathfrak{h}}\langle \mathrm{e}_x,\Theta_{s_1,\ell}\mathrm{e}_y\rangle_{\mathfrak{h}}\langle \mathrm{e}_z,h^{(\omega)}\mathrm{e}_w\rangle_{\mathfrak{h}}\left\langle \mathrm{e}^{i(s_1-t)h^{(\omega)}}\mathrm{e}_y,\mathrm{e}_z\right\rangle_{\mathfrak{h}}$$
$$\times\left(\langle \mathrm{e}^{is_2h^{(\omega)}}\mathrm{e}_v,\mathrm{e}^{is_1h^{(\omega)}}\mathrm{e}_x\rangle_{\mathfrak{h}}\left\langle \mathrm{e}_w,\frac{\mathrm{e}^{i(s_2-t)h^{(\omega)}}}{1+\mathrm{e}^{\beta h^{(\omega)}}}\mathrm{e}_u\right\rangle_{\mathfrak{h}}-\langle \mathrm{e}^{ith^{(\omega)}}\mathrm{e}_w,\mathrm{e}^{is_2h^{(\omega)}}\mathrm{e}_u\rangle_{\mathfrak{h}}\left\langle \mathrm{e}_v,\frac{\mathrm{e}^{i(s_1-s_2)h^{(\omega)}}}{1+\mathrm{e}^{\beta h^{(\omega)}}}\mathrm{e}_x\right\rangle_{\mathfrak{h}}\right)$$
$$+\frac{i}{|\mathcal{R}_\ell|}\sum_{x,y,u,v\in\mathbb{Z}^d}\sum_{z,w\in\mathcal{R}_\ell}\langle \mathrm{e}_u,\Theta_{s_2,\ell}\mathrm{e}_v\rangle_{\mathfrak{h}}\langle \mathrm{e}_y,\Theta_{s_1,\ell}\mathrm{e}_x\rangle_{\mathfrak{h}}\langle \mathrm{e}_w,h^{(\omega)}\mathrm{e}_z\rangle_{\mathfrak{h}}\left\langle \mathrm{e}_z,\mathrm{e}^{i(s_1-t)h^{(\omega)}}\mathrm{e}_y\right\rangle_{\mathfrak{h}}$$
$$\times\left(\langle \mathrm{e}^{ith^{(\omega)}}\mathrm{e}_x,\mathrm{e}^{is_2h^{(\omega)}}\mathrm{e}_u\rangle_{\mathfrak{h}}\left\langle \mathrm{e}_v,\frac{\mathrm{e}^{i(s_1-s_2)h^{(\omega)}}}{1+\mathrm{e}^{\beta h^{(\omega)}}}\mathrm{e}_w\right\rangle_{\mathfrak{h}}-\langle \mathrm{e}^{is_2h^{(\omega)}}\mathrm{e}_v,\mathrm{e}^{is_1h^{(\omega)}}\mathrm{e}_w\rangle_{\mathfrak{h}}\left\langle \mathrm{e}_x,\frac{\mathrm{e}^{i(s_2-t)h^{(\omega)}}}{1+\mathrm{e}^{\beta h^{(\omega)}}}\mathrm{e}_u\right\rangle_{\mathfrak{h}}\right)$$

which equals

$$\begin{aligned}\varrho^{(\omega)}(\mathbf{K}) &= \frac{i}{|\mathcal{R}_\ell|}\mathrm{Tr}_{\mathfrak{h}}\left(\mathrm{e}^{i(t-s_1)h^{(\omega)}}P_{\mathcal{R}_\ell}h^{(\omega)}P_{\mathcal{R}_\ell}\frac{\mathrm{e}^{i(s_2-t)h^{(\omega)}}}{1+\mathrm{e}^{\beta h^{(\omega)}}}\Theta_{s_2,\ell}\mathrm{e}^{i(s_1-s_2)h^{(\omega)}}\Theta_{s_1,\ell}\right)\\&\quad-\frac{i}{|\mathcal{R}_\ell|}\mathrm{Tr}_{\mathfrak{h}}\left(\mathrm{e}^{i(t-s_1)h^{(\omega)}}P_{\mathcal{R}_\ell}h^{(\omega)}P_{\mathcal{R}_\ell}\mathrm{e}^{i(s_2-t)h^{(\omega)}}\Theta_{s_2,\ell}\frac{\mathrm{e}^{i(s_1-s_2)h^{(\omega)}}}{1+\mathrm{e}^{\beta h^{(\omega)}}}\Theta_{s_1,\ell}\right)\\&\quad\frac{i}{|\mathcal{R}_\ell|}\mathrm{Tr}_{\mathfrak{h}}\left(\Theta_{s_1,\ell}\mathrm{e}^{i(s_2-t)h^{(\omega)}}\Theta_{s_2,\ell}\frac{\mathrm{e}^{i(s_1-s_2)h^{(\omega)}}}{1+\mathrm{e}^{\beta h^{(\omega)}}}P_{\mathcal{R}_\ell}h^{(\omega)}P_{\mathcal{R}_\ell}\mathrm{e}^{i(s_1-t)h^{(\omega)}}\right)\\&\quad-\frac{i}{|\mathcal{R}_\ell|}\mathrm{Tr}_{\mathfrak{h}}\left(\Theta_{s_1,\ell}\frac{\mathrm{e}^{i(s_2-t)h^{(\omega)}}}{1+\mathrm{e}^{\beta h^{(\omega)}}}\Theta_{s_2,\ell}\mathrm{e}^{i(s_1-s_2)h^{(\omega)}}P_{\mathcal{R}_\ell}h^{(\omega)}P_{\mathcal{R}_\ell}\mathrm{e}^{i(s_1-t)h^{(\omega)}}\right).\end{aligned}$$

Using the cyclicity of the trace, this equation can be rewritten as

$$\begin{aligned}\varrho^{(\omega)}(\mathbf{K}) = & \frac{i}{|\mathcal{R}_\ell|}\mathrm{Tr}_{\mathfrak{h}}\left(P_{\mathcal{R}_\ell} h^{(\omega)} P_{\mathcal{R}_\ell} \mathrm{e}^{i(s_2-t)h^{(\omega)}} \mathfrak{Q}_{s_2,\ell}^{(\omega)} \mathrm{e}^{i(s_1-s_2)h^{(\omega)}} \Theta_{s_1,\ell} \mathrm{e}^{i(t-s_1)h^{(\omega)}}\right) \\ & - \frac{i}{|\mathcal{R}_\ell|}\mathrm{Tr}_{\mathfrak{h}}\left(\Theta_{s_1,\ell} \mathrm{e}^{i(s_2-t)h^{(\omega)}} \mathfrak{Q}_{s_2,\ell}^{(\omega)} \mathrm{e}^{i(s_1-s_2)h^{(\omega)}} P_{\mathcal{R}_\ell} h^{(\omega)} P_{\mathcal{R}_\ell} \mathrm{e}^{i(s_1-t)h^{(\omega)}}\right)\end{aligned}$$

with

$$\mathfrak{Q}_{s_2,\ell}^{(\omega)} := \left[\left(1+\mathrm{e}^{\beta h^{(\omega)}}\right)^{-1}, \Theta_{s_2,\ell}\right].$$

■

This time derivative of the function

$$t \mapsto \varrho^{(\omega)}\left(\mathbf{Z}_{\ell,t}^{(\omega,\mathbf{A})}\right)$$

can directly be computed on the one-particle Hilbert space $\mathfrak{h}$, by using Lemma 7.8.4. It can also be done in the CAR C^*-algebra:

$$\begin{aligned}\partial_t \mathbf{Z}_{\ell,t}^{(\omega,\mathbf{A})} = & -\eta^{-2}\int_0^t \mathrm{d}s \left(\left[\tau_s^{(\omega)}\left(W_s^{(\eta\mathbf{A}_\ell)}\right), \tau_t^{(\omega)}\left(W_t^{(\eta\mathbf{A}_\ell)}\right), \tau_t^{(\omega)}(\mathfrak{E}_{\mathcal{R}_\ell}^{(\omega)}))\right]^{(3)}\right) \\ & - \eta^{-2}\int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \left(\left[\tau_{s_2}^{(\omega)}\left(W_{s_2}^{(\eta\mathbf{A}_\ell)}\right), \tau_{s_1}^{(\omega)}\left(W_{s_1}^{(\eta\mathbf{A}_\ell)}\right), \partial_t \tau_t^{(\omega)}(\mathfrak{E}_{\mathcal{R}_\ell}^{(\omega)}))\right]^{(3)}\right)\end{aligned}$$

and if $\{W_t^{(\eta\mathbf{A}_\ell)}\}_{t\geq 0}$ is a cyclic process of length T (see Definition 2.1.2), we obtain that, for $t \geq T$,

$$\partial_t \mathbf{Z}_{\ell,t}^{(\omega,\mathbf{A})} = -\eta^{-2}\int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \left(\left[\tau_{s_2}^{(\omega)}\left(W_{s_2}^{(\eta\mathbf{A}_\ell)}\right), \tau_{s_1}^{(\omega)}\left(W_{s_1}^{(\eta\mathbf{A}_\ell)}\right), \partial_t \tau_t^{(\omega)}(\mathfrak{E}_{\mathcal{R}_\ell}^{(\omega)}))\right]^{(3)}\right) \tag{7.99}$$

with $\partial_t \tau_t^{(\omega)}(B)$ being defined for any $B \in \mathcal{U}_0$ as follows: Recall that $\{\tau_t^{(\omega)}\}_{t\in\mathbb{R}}$ is a strongly continuous group of $*$-automorphisms of $\mathcal{U}$, and, by the semigroup theory (Section 8.2), it has a (unbounded) infinitesimal generator $\delta^{(\omega)}$ acting on $\mathcal{U}$. Similar to Proposition 3.2.7 in the finite-volume case, one infers from [31, Theorem 4.8] that δ is a conservative closed symmetric derivation which is equal on its core $\mathcal{U}_0$ to

$$\delta(B) = i\sum_{x,y\in\mathbb{Z}^d} \langle \mathfrak{e}_x, h^{(\omega)}\mathfrak{e}_y\rangle_{\mathfrak{h}} \left[a^*(\mathfrak{e}_x)a(\mathfrak{e}_y), B\right], \qquad B \in \mathcal{U}_0,$$

where we recall that $\mathcal{U}_0$ is the $*$-algebra of local elements of $\mathcal{U}$ defined by (4.16). In particular, the integrand in (7.99) is a multicommutator of order 4. By using Lieb Robinson bound for multi-commutators (or tree-decay bounds [31, Corollary 4.12] in this case), one can again obtain that

$$\partial_t \mathbf{Z}_{\ell,t}^{(\omega,\mathbf{A})} = \mathcal{O}(1),$$

uniformly with respect to $\omega \in \Omega$, $\lambda, \ell \in \mathbb{R}_0^+$ and t in compact sets. Another way to compute $\partial_t \tau_t^{(\omega)}(\mathfrak{E}_{\mathcal{R}_\ell}^{(\omega)})$ in the integrand in Equation (7.99) in order to show that last property is to use the quasi-free property of the dynamics, which implies that, for any $x \in \mathbb{Z}^d$, $\omega \in \Omega$, and $t \in \mathbb{R}$,

$$\partial_t \tau_t^{(\omega)}(a(\mathfrak{e}_x)) = \partial_t a(\mathrm{e}^{ith^{(\omega)}} \mathfrak{e}_x) = a(\partial_t(\mathrm{e}^{ith^{(\omega)}} \mathfrak{e}_x)) = a(i\mathrm{e}^{ith^{(\omega)}} h^{(\omega)} \mathfrak{e}_x)) = -ia(\mathrm{e}^{ith^{(\omega)}} h^{(\omega)} \mathfrak{e}_x)),$$

because of the fact that

$$\|a(\psi)\|_{\mathcal{U}} = \|\psi\|_{\mathfrak{h}}, \qquad \psi \in \mathfrak{h}.$$

See, e.g., Proposition 3.1.5.

Chapter 8

Appendix

8.1 Appendix 1: Mathematical foundation

Within this appendix, we discuss about the mathematical foundation of the construction that are involved to give sense to the algebraic formulation of quantum mechanics. It can be useful to motivate the use of C^*-algebra to formulate quantum problem. This appendix is directly taken from the lecture notes of Prof. J.B. Bru, see [90]. Note that, we cite some results and remark on C^*-algebra without the proofs, for more details, see [26] and [27]. Indeed, those books are widely considered and used in order to learn the algebraic formulation of Quantum Statistical Mechanics.

Definition 8.1.1 (Observables)
A physical system $\mathcal{S}$ is described by its physical properties, i.e., by a non-empty set $\mathcal{O}$ of quantities that can be measured within $\mathcal{S}$ as well as their relations between each other. An element A of $\mathcal{O}$ is called an observable.

Axiom 1
For any observable A, its measure is contained within a bounded set denoted by $W_A \subset \mathbb{R}$.

Axiom 2
If A is an observable and $P \in \mathbb{R}[X]$ (a polynomial with real coeficients), then there exists an observable $P(A)$. Moreover, for two polynomials P_1 and P_2, with real coefficients, then

$$P_1(P_2(A)) = P_1 \circ P_2(A) \quad \text{and} \quad (P_1 + P_2)(A) = P_1(A) + P_2(A), \quad \text{for all } A \in \mathcal{O}.$$

with

$$P_1(P_2(x)) = P_1 \circ P_2(x) \quad \text{and} \quad (P_1 + P_2)(x) = P_1(x) + P_2(x), \quad \text{for all } x \in \mathbb{R}.$$

For instance, for any *observable* A, let $P_1(x) := \lambda x$ and $P_2(x) := x^n$ for $\lambda, x \in \mathbb{R}$ and $n \in \mathbb{N}$. Then

$$P_1(A) = \lambda A \quad \text{and} \quad P_2(A) = A^n.$$

Axiom 3
For all observable A and all polynomial $P \in \mathbb{R}[X]$ with real coefficient

$$W_{P(A)} = P(W_A) := \{P(x) : x \in W_A\}.$$

Lemma 8.1.2
For all $\lambda \in \mathbb{R}$, there is an observable $\boldsymbol{\lambda}$ such that $W_{\boldsymbol{\lambda}} = \{\lambda\}$.

Proof: From Axiom 2, for any *observable A*, let us define $\boldsymbol{\lambda} := P(A)$, where $P(x) = \lambda$ for all $x \in \mathbb{R}$. By using Axiom 3,

$$W_{\boldsymbol{\lambda}} := W_{P(A)} := \{P(x) : x \in W_A\} = \lambda.$$

Note that at this point, $W_{\boldsymbol{\lambda}} = \{\lambda\}$ can be deduced from an infinite numbers of *observables*. ■

Definition 8.1.3
A state ρ is a map from $\mathcal{O}$ to $\mathbb{R}$ and represents the statistical distribution of all measures of any observables. The set of states is denoted by E.

Remark 8.1.4
$\rho(A)$ is the expectation value of the measurement of an observable A when the physical system is in the state ρ.

Definition 8.1.5
A state ρ is said to be dispersion free with respect to an observable A if there exists a unique value $a \in \mathbb{R}$ such that

$$\rho(A) = a \in W_A \quad \text{and} \quad \rho(P(A)) = P(A), \quad \forall P \in \mathbb{R}[X].$$

The set of dispersion free state with respect to an observable A is denoted by E^A.

Obviously, from Axioms 2-3, it follows that $E^A \subset E^{P(A)}$ for all $P \in \mathbb{R}[X]$ and $A \in \mathcal{O}$. Moreover, $\rho(\boldsymbol{\lambda}) = \lambda$ for all $\lambda \in \mathbb{R}$ and $\rho \in E$. This motivates the next axiom:

Axiom 4
For any observable A, any state ρ and $\lambda \in \mathbb{R}$,

- $\inf W_A \le \rho(A) \le \sup W_A$.
- $\rho(\lambda A) = \lambda \rho(A)$.

Remark 8.1.6
From Axioms 2-3-4, for all $\boldsymbol{\lambda} \in \mathcal{O}$ such that $W_{\boldsymbol{\lambda}} = \{\lambda\}$ with $\lambda \in \mathbb{R}$, $E^{\boldsymbol{\lambda}} = E$.

Definition 8.1.7 (Spectrum of observables)
The spectrum of all $A \in \mathcal{O}$ is defined by

$$\sigma(A) := \left\{\rho(A) : \rho \in E^A\right\} \subset \mathbb{R}.$$

Note that from Axiom 4, one has that, for any *observable* A, $\sigma(A) \subset W_A$. Moreover, for all $P \in \mathbb{R}[X]$,

$$P(\sigma(A)) \subset (P(A)) \subset P(W_A).$$

Axiom 5 (Spectrum as possible measures)
For all $A \in \mathcal{O}$, $\sigma(A) = W_A$. In other words, the spectrum of an observable A is the set of all possible measure of the physical quantity A.

Definition 8.1.8 (Order of observables)
For all $A, B \in \mathcal{O}$, if $\rho(A) \geq \rho(B)$ for all $\rho \in E$, the one says that $A \geq B$.

Note that, at this point, $A \geq B$ and $B \geq C$ implies that $A \geq C$, for all *observables* A, B, C. The next axiom clarifed the anisymmety of this order relation:

Axiom 6 (States separate observables)
If $A \geq B$ and $B \geq A$, the $A = B$. In particular, the order $\geq$ defines a partial order in $\mathcal{O}$.

Note that form Axioms 2-3-4-6, For all $\lambda \in \mathbb{R}$, the set $W_{\boldsymbol{\lambda}} := \{\lambda\}$ defines a unique *observable* $\boldsymbol{\lambda}$. Therefore, the set of *observables* includes $\mathbf{0}$ and $\mathbf{1}$, which are the *observables* such that their measures are respectively $0 = W_{\mathbf{0}}$ and $1 = W_{\mathbf{1}}$.

Definition 8.1.9 (Positive *observables*)
An observable A is said to be positive when $A \geq \mathbf{0}$.

Lemma 8.1.10
Assume Axioms 2-6. Then $A \in \mathcal{O}$ is positive if and only if $W_A \subset \mathbb{R}_0^+$.

Proof: Obvious. ■

Axiom 7
For all $A, B \in \mathcal{O}$, there is an observable $A + B \in \mathcal{O}$ such that $\rho(A + B) = \rho(A) + \rho(B)$ for all $\rho \in E$.

Remark 8.1.11
From Axiom 6, $A + B \in \mathcal{O}$ is unique. Moreover, since

$$\rho(A + \mathbf{0}) = \rho(A) + \rho(\mathbf{0}) = \rho(A), \quad \textit{for all } \rho \in E.$$

Then,

$$A + \mathbf{0} = \mathbf{0} + A = A, \quad \textit{for all } A \in \mathcal{O}.$$

Theorem 8.1.1
Assume Axioms 2-7. Then, $(\mathcal{O}, +, \cdot)$ *is a real vector space.*

Proof: $(\mathcal{O}, +)$ is an abelian group with a neutral element $\mathbf{0}$ (see Remark 8.1.11). Indeed, for all $A, B, C \in \mathcal{O}$, $\rho \in E$ and $\lambda \in \mathbb{R}$, from Axiom 7, the *observables* $A + B$ and $B + A$ satisfy

$$\rho(A + B) = \rho(A) + \rho(B) = \rho(B) + \rho(A) = \rho(B + A).$$

In other words

$$A + B = B + A.$$

Moreover, from Axiom 7, the *observables* $(A + B) + C$ and $A + (B + C)$ satisfy

$$\rho\left((A + B) + C\right) = \rho(A + B) + \rho(C) = \rho(A) + \rho(B) + \rho(C) = \rho(A) + \rho(B + C) = \rho\left(A + (B + C)\right).$$

In other words

$$(A + B) + C = A + (B + C) \quad \text{(associativity)}.$$

Furthermore, if one defines $-A := (-1)A \in \mathcal{O}$ (by using Axiom 4). Then

$$\rho\left((-1)A + A\right) = -\rho(A) + \rho(A) = 0 = \rho(\mathbf{0}).$$

In other words, $-A$ is the inverse of A. Finally,

$$\rho(\lambda(A + B)) = \lambda\rho(A + B) = \lambda(\rho(A) + \rho(B)) = \lambda\rho(A) + \lambda\rho(B).$$

In other words,

$$\lambda(A + B) = \lambda A + \lambda B \quad \text{(distributivity)}.$$

■

Definition 8.1.12 (Norm of *observables*)
For all $A \in \mathcal{O}$,

$$\|A\| = \sup_{\rho \in E} \left|\rho(A)\right|.$$

By using Axioms 1, 4 anf 5, one has, for all $A \in \mathcal{O}$

$$\|A\| = \sup_{x \in W_A} \{|x|\} = \sup_{x \in \sigma(A)} \{|x|\}.$$

Theorem 8.1.2
Assume Axioms 1-7. Then, $(\mathcal{O}, \|\cdot\|, +, \cdot)$ *is a normed vector space.*

Proof: For all $\lambda \in \mathbb{R}$, $\rho \in E$ and $A, B \in \mathcal{O}$. One has,

$$|\rho(\lambda A)| = |\lambda||\rho(A)|.$$

Which means that

$$||\lambda A|| = |\lambda|||A||.$$

Moreover, $||A|| = 0$ if and only if $\rho(A) = \rho(\mathbf{0})$, for all $\rho \in E$. Which means that

$$||A|| = 0 \text{ if and only if } A = \mathbf{0}.$$

Finally, the triangle inequality is obvious by writing

$$||A + B|| = \sup_{\rho \in E}(|\rho(A) + \rho(B)|) \leq \sup_{\rho \in E}|\rho(A)| + \sup_{\rho \in E}|\rho(B)| = ||A|| + ||B||.$$

■

Theorem 8.1.3 (C^*-property of the norm)
Assume Axioms 1-7. Then, for all $A \in \mathcal{O}$, $||A^2|| = ||A||^2$.

Proof: First, note that from the definition of the norm of *observables* given above, one has

$$W_{-A} \cup W_A \subset [-||A||, ||A||] .$$

Let $C := A^2$, $B := ||A||^2\mathbf{1} - A^2$ and $P_1, P_2 \in \mathbb{R}[X]$ such that

$$P_1(x) := (||A|| - x)(||A|| + x) \quad \text{and} \quad P_2(x) := x^2$$

In particular, note that

$$P_1(A) = B, \quad \text{and} \quad P_2(A) = C.$$

By using Axiom 3, on has

$$W_B = W_{P_1(A)} = P_1(W_A) \subset P([-||A||, ||A||]) \subset \mathbb{R}_0^+ \text{ and}$$

$$W_C = W_{P_2(A)} = P_2(W_A) \subset \mathbb{R}_0^+$$

Therefore, from Lemma 8.1.10, $B \geq \mathbf{0}$ and $C \geq \mathbf{0}$. In particular,

$$||A||^2 \geq \rho(A^2) = \rho(C) \geq 0, \quad \text{for all } \rho \in E.$$

This implies that,

$$||A||^2 \geq ||A^2||.$$

Now let $D := ||A||^2 - 2||A||A + A^2$ and $P_3 \in \mathbb{R}[X]$ such that for all $x \in \mathbb{R}$

$$P_3(x) = (x - ||A||)^2.$$

In the same way as previously, $D \geq \mathbf{0}$ which means that

$$2\|A\||\rho(A)| \leq \|A\|^2 + \rho(A^2) \leq \|A\|^2 + \|A^2\|, \quad \text{for all } \rho \in E.$$

This implies that,

$$\|A\|^2 \leq \|A^2\|.$$

■

Axiom 8
The normed vector space $(\mathcal{O}, \|\cdot\|)$ is complete.

Hitherto, $\mathcal{O}$ is a banach space. In particular, its dual is well defined:

Definition 8.1.13
$\mathcal{O}^*$ is the set of all continuous $\mathbb{R}$-linear functionals from $\mathcal{O}$ to $\mathbb{R}$.

Remark 8.1.14
The notation $\mathcal{O}^*$ is introduced here in the appendix, we try to avoid this all along the manuscript of the thesis to avoid any confusion such as the adjoint operator for instance.

A linear map ρ from $\mathcal{O}$ to $\mathbb{R}$ is continuous if and only if

$$\|\rho\| := \sup_{A \in \mathcal{O}: \|A\| \leq 1} |\rho(A)| < \infty.$$

Definition 8.1.15
$\rho \in \mathcal{O}^*$ is positive if $\rho(A) \geq 0$ for all $A \geq \mathbf{0}$, $A \in \mathcal{O}$. The set of all positive continuous $\mathbb{R}$-linear functionals is denoted by $\mathcal{O}^*_+$. Furthermore, $\rho \in \mathcal{O}^*$ is normalized if $\rho(\mathbf{1}) = 1$. The set of all normalized continuous $\mathbb{R}$-linear functionals is denoted by $\mathcal{O}^*_+$ is denoted by $\mathcal{O}^*_1$. This allows us to define the set of all positive, normalized continuous $\mathbb{R}$-linear functionals

$$\mathcal{O}^*_{+,1} := \mathcal{O}^*_1 \cap \mathcal{O}^*_+.$$

Axiom 9 (*Observables* separate states)
Let $\rho_1, \rho_2 \in E$. If $\rho_1(A) = \rho_2(A)$, for all $A \in \mathcal{O}$, then $\rho_1 = \rho_2$.

Lemma 8.1.16
Assume Axioms 1-9. Then, $E \subseteq \mathcal{O}^*_{+,1}$. In other words, states are positive normalized continuous $\mathbb{R}$-linear functionals.

Proof: Obvious. ■

This leads us to the next axiom:

Axiom 10
We assume that $E = \mathcal{O}^*_{+,1}$.

Note that it is easy to see that for any $\alpha \in [0,1]$ and $\rho_1, \rho_2 \in \mathcal{O}^*_{+,1}$,

$$\alpha\rho_1 + (1-\alpha)\rho_2 \in \mathcal{O}^*_{+,1}.$$

It means that $\mathcal{O}^*_{+,1}$ is a convex set.

Definition 8.1.17 (Symmetric product)
Under Axioms 2-7, define the operation $\bullet_s$ from $\mathcal{O} \times \mathcal{O}$ to $\mathcal{O}$ by

$$(A,B) \mapsto A \bullet_s B := \frac{1}{2}\left((A+B)^2 - A^2 - B^2\right).$$

Remark 8.1.18
One can easily see that, for all $A, B \in \mathcal{O}$:

- $A \bullet_s B = B \bullet_s A$,
- $A \bullet_s \mathbf{0} = \mathbf{0}$,
- $A \bullet_s \mathbf{1} = \mathbf{1}$.

Axiom 11 (Homogeneity)
The operation $\bullet_s$ is homogeneous with respect to the first argument, i.e., for all $A, B \in \mathcal{O}$ and $\lambda \in \mathbb{R}$

$$(\lambda A) \bullet_s B = \lambda\,(A \bullet_s B)\,.$$

Remark 8.1.19
The homogeneity of the operation $\bullet_s$ with respect to the second argument is also satisfied because of Remark 8.1.18.

We cite now two results of which we do not give formal proofs. Indeed, the can easily be obtained by direct computation assuming previous results.

Theorem 8.1.4
Assume Axioms 2-11. Then, $(\mathcal{O}, +, \bullet_s)$ is a distributive an commutative algebra, i.e., for all $A, B, C \in \mathcal{O}$,

$$(A+B) \bullet_s C = A \bullet_s C + B \bullet_s C.$$

Theorem 8.1.5 (Continuity of $\bullet_s$ and $()^2$ in $\mathcal{O}$)
Assume Axioms 1-11. Then, for all $A, B, \in \mathcal{O}$,

- $\|A \bullet_s B\| \leq \|A\|\|B\|$.
- $\|A^2 - B^2\| \leq \max\{\|A\|^2, \|B\|^2\}\,.$
- *If there exists a sequence $(A_n)_{n\in\mathbb{N}} \in \mathcal{O}$ such that $A_n \to A$ in $(\mathcal{O}, \|\cdot\|)$. Then, $A_n^2 \to A^2$ in $(\mathcal{O}, \|\cdot\|)$.*

Note that formally, $A \bullet_s B = \frac{1}{2}(AB + BA)$. The problem is that the product AB depends on the physical system that is considered.

At this point, we did not yet see the reason to use the framework of C^*-algebra. We fill now the gap by introducing this concept and motivate the fact that a C^*-algebra satisfies Axioms 1-10. Consider a unital C^*-algebra $\mathcal{X} := (\mathcal{X}, \|\cdot\|, \cdot, *, +)$.

Remark 8.1.20 *The set of all self-adjoint elements of $\mathcal{X}$ is denoted by*

$$\mathcal{O}_{\mathcal{X}} =: \{A \in \mathcal{X} : A = A^*\} .$$

It is easy to check that $(\mathcal{O}_{\mathcal{X}}, +, \cdot)$ is a real vector space, see Theorem 8.1.1. Moreover, A is invertible if and only if A^* is invertible and

$$(A^{-1})^* = (A^*)^{-1}.$$

Definition 8.1.21 (Resolvent)
For $A \in \mathcal{X}$, the resolvent is defined as

$$\varrho(A) =: \{\lambda \in \mathbb{C} : (\lambda \mathbf{1} - A) \text{ is invertible}\} .$$

The spectrum of A is $\sigma(A) := \mathbb{C} \setminus \varrho(A)$.

Proposition 8.1.22 (Spectral radius)
Let A be an element of a unital Banach algebra, then

$$r(A) \leq \|A\|$$

where

$$r(A) := sup \{|\lambda| : \lambda \in \sigma(A)\}$$

is the spectral radius of A.

Proof: Suppose that $|\lambda| > \|A\|$, it is clear that

$$\lambda^{-1} \sum_{m \geq 0} \left(\frac{A}{\lambda}\right)^m$$

converges and by completeness of the Banach algebra, it defines an element that is $(\lambda \mathbf{1} - A)^{-1}$. Hence ,by definition, $\lambda \in \varrho(A)$ and

$$\sigma(A) \subseteqq \{\lambda \in \mathbb{C} : |\lambda| \leq \|A\|\}.$$

This concludes the proof. ∎

Standard results of spectral theory set that (see for instance [27]),

Theorem 8.1.6 (Spectrum in C^*-algebras)
For $A \in \mathcal{X}$, then

i) $r(A) = \lim_{n\to\infty} \|A^n\|^{\frac{1}{n}}$ *(which means that the spectrum of A is not an empty set).*

ii) *If $A^*A = AA^*$, then $r(A) = \|A\|$.*

iii) *If $A^*A = AA^* = \mathbf{1}$, then $r(A) = 1$.*

iv) *If $A \in \mathcal{O}_{\mathcal{A}}$, then $\sigma(A) \in [-\|A\|, \|A\|]$ and $\sigma(A^2) \in [0, \|A\|^2]$.*

v) *For a polynomial $P \in \mathbb{C}[X]$*

$$\sigma(P(A)) = P(\sigma(A)) := \{P(\lambda) : \lambda \in \sigma(A)\}.$$

Remark 8.1.23
$\sigma(A) \in \mathbb{R}$, for $A \in \mathcal{X}$ such that $A = A^*$. Furthermore, for any $P \in \mathbb{R}[X]$, $\sigma(P(A)) = P(\sigma(A))$. See Axiom 3.

Definition 8.1.24 (Positive elements)
An element A of $\mathcal{X}$ is positive if $A = A^*$ and $\sigma(A)$ is a subset of $\mathbb{R}_0^+$, compare with Lemma 8.1.10. The set of all positive elements will be noted $\mathcal{X}^+$.

Note that $\mathcal{X}^+$ is a closed set in $\mathcal{X}$ with $\mathbf{0} \in \mathcal{X}^+$. Furthermore, by [26, Theorem 2.2.12],

Theorem 8.1.7 (Positive elements)
Let $A \in \mathcal{X}$. The following conditions are equivalent:

i) *A is positive.*

ii) *There exists a (non trivial) element $B \in \mathcal{X}$ such that*

$$A = B^*B.$$

Definition 8.1.25 (Order relation)
Let $A, B \in \mathcal{X}$. $A \geq B$ if $A - B \in \mathcal{X}^+$.

Lemma 8.1.26
The relation $\geq$ is a partial order in $\mathcal{X}$, compare with Axiom 6.

Proof: The reflexivity of $\geq$ follows from the fact that $\mathbf{0} \in \mathcal{X}^+$. Furthermore, if $A, B \in \mathcal{X}^+$, then $A + B \in \mathcal{X}^+$ (actually, $\mathcal{X}^+$ is a cone). This implies the transitivity of $\geq$. Now let $A, B \in \mathcal{X}$ such that $A \geq B$ and $B \geq A$. Then,

$$(A - B) \in \mathcal{X}^+ \quad \text{and} \quad (B - A) = -(A - B) \in \mathcal{X}^+.$$

Therefore,

$$\sigma(A - B) \in \mathbb{R}_0^+ \quad \text{and} \quad \sigma(-(A - B)) \in \mathbb{R}_0^+.$$

Define the $P \in \mathbb{R}[X]$, such that $P(x) := -x$. Hence, by applying Theorem 8.1.6, it follows that

$$\sigma(A - B) = \{0\}.$$

This implies that

$$\|A - B\| = 0.$$

■

We introduce now the concept of states of C^*-algebra. Here ρ is a continuous linear functional from $\mathcal{X}$ to $\mathbb{C}$.

Definition 8.1.27 (Hermitian and positivity)
We give now the definition of state,

1. *ρ is Hermitian if*

$$\rho(A) = \overline{\rho(A^*)}, \quad \forall A \in \mathcal{X}.$$

2. *ρ is positive if $\rho(A) \geq 0$, for all $A \in \mathcal{X}^+$. A positive state is denoted by $\rho \geq 0$.*

Note that, by [26, Section 2.2.2], for any $A \in \mathcal{X}^+$, there exists a non-trivial element of B of $\mathcal{X}$ such that $A = B^*B$. Conversely, for any $B \in \mathcal{X}$, $B^*B \in \mathcal{X}^+$. We are now in position to give the following result:

Lemma 8.1.28
Let $A \in \mathcal{X}$ such that $A = A^*$. If $\rho \geq 0$, then

$$\rho(B^*AB) \leq \|A\|\rho(B^*B).$$

Proof: Observe that, by Theorem 8.1.6, $\sigma(A) \in [-\|A\|, \|A\|]$. Note that,

$$\|A\|B^*B - B^*AB = B^*(\|A\| - A)B.$$

Let

$$C := \|A\| - A$$

and define $P \in \mathbb{R}[X]$ such that $P(x) = \|A\| - x$. Clearly, $C^* = C = P(A)$. By using Theorem 8.1.6, one has

$$\sigma(C) = \sigma(P(A)) = P(\sigma(A)) \subset \mathbb{R}_0^+.$$

It follows that $C \in \mathcal{X}^+$. Then, there is a element $D \in \mathcal{X}$ such that $C = D^*D$. Therefore,

$$\|A\|B^*B - B^*AB = B^*D^*DB.$$

Which implies that

$$\|A\|B^*B - B^*AB \in \mathcal{X}^+,$$

this yields the Lemma ■

We are now in position to define states on a C^*-algebra.

Definition 8.1.29 (State)
A state is a positive, normalized linear functional from $\mathcal{X}$ to $\mathbb{C}$. In other words, ρ is a state if,

$$\rho(B^*B) \geq 0, \quad \text{for all } B \in \mathcal{X} \quad \text{and} \quad \|\rho\| = \rho(\mathbf{1}) = 1.$$

The set of states is denoted by $\mathcal{X}^*_{+,1}$.

Remark 8.1.30 (States separates points)
From [26], we can also mention the following results, for $A \in \mathcal{X}$,

- $\rho(A) = 0$, *for all $\rho \in \mathcal{X}^*_{+,1}$, imply that $A = \mathbf{0}$.*
- $\rho(A) \in \mathbb{R}$, *for all $\rho \in \mathcal{X}^*_{+,1}$, yields $A^* = A$.*
- $\rho(A) \geq 0$, *for all $\rho \in \mathcal{X}^*_{+,1}$, yields $A^* \in \mathcal{X}^+$.*
- $AA^* = A^*A$ *implies that there is $\rho \in \mathcal{X}^*_{+,1}$ such that $|\rho(A)| = \|A\|$.*

Definition 8.1.31 (Spectrum of a C^*-algebra) *A linear functional $\rho : \mathcal{X} \to \mathbb{C}$ is a character if, for all $A, B \in \mathcal{X}$,*

$$\rho\,(AB) = \rho\,(A)\,\rho\,(A)\,.$$

The set $\sigma(\mathcal{X})$ of all character of $\mathcal{X}$ is called the spectrum of $\mathcal{X}$.

Lemma 8.1.32
If $\mathcal{X}$ is a commutative C^*-algebra, then $\sigma(\mathcal{X}) \subset \mathcal{X}^*_{+,1}$. Moreover, for all $\rho \in \sigma(\mathcal{X})$ and $A \in \mathcal{X}$, $\rho(A) \in \sigma(A)$.

Theorem 8.1.8
If $\mathcal{X}$ is a commutative C^*-algebra and $A \in \mathcal{X}$. Then, for all $a \in \sigma(A)$, there is $\rho \in \sigma(\mathcal{X})$ such that $\rho(A) = a$.

As a conclusion, note that the set of self-adjoint elements of a C^*-algebra is not the unique structure from which one can obtain the mathematical foundation of quantum mechanics. However, we consider the formulation relying on C^*-algebras in the context of this thesis. Indeed, on can see that

- The set of *observables:*
$$\mathcal{O} := \mathcal{O}_{\mathcal{X}}.$$
- The set of states:
$$E = \mathcal{O}^*_{\mathcal{X},+,1} := \mathcal{X}^*_{+,1}.$$
- For all $A \in \mathcal{O}$, let $W_A := \sigma(A) \subset \mathbb{R}$.
- For all $P \in \mathbb{R}\,[X]$, $P(x) := \sum_{k=0}^{n} c_k x^k$. Then, for all $A \in \mathcal{O}$,
$$P(A) := \sum_{k=0}^{n} c_k A^k \in \mathcal{O},$$

and Axioms 1-11 holds for $\mathcal{X} := (\mathcal{X}, \|\cdot\|, \cdot, *, +)$.

8.2 Appendix 2: Semigroup theory

Within this appendix, we present the main results on semigroup theory in order to give a sense to the time evolution in quantum mechanics. This apendix is highly inspired by [41].

Semigroups and Generators

First of all, let us give the definitions and basic results of semigroup theory as it is given in [41]. These will provide the basis required to prove the main theorems studied in this article. Let X be a Banach space.

Definition 8.2.1 *A strongly continuous one-parameter semigroup, also called C^0-semigroup, is a family $(T(t))_{t\geq 0}$ of bounded operators $T : X \to X$ satisfying the functional equation*

$$\begin{cases} T(t+s) = T(t)T(s) \text{ for all } t, s \geq 0, \\ T(0) = \mathbf{1}_X \end{cases}$$

and the strong continuity property, which is nothing else but the continuity of the orbit maps

$$\begin{array}{rcl} \xi_x : \mathbb{R}^+ & \longrightarrow & X \\ t & \longmapsto & \xi_x(t) := T(t)x \end{array}$$

for each $x \in X$. If these properties hold not only in $\mathbb{R}^+$ but also in $\mathbb{R}$, we call $(T(t))_t$ a strongly continuous group, or C^0-group.

Lemma 8.2.2 *Let $(T(t))_{t\geq 0}$ be a C^0-semigroup. Then, there exist $\omega \in \mathbb{R}$ and $M \geq 1$ such that, for all $t \geq 0$,*

$$\|T(t)\|_{\mathcal{B}(X)} \leq M\,\mathrm{e}^{\omega t}.$$

Proof: From the uniform boundedness, there exists $M \geq 1$ such that $\|T(s)\|_{\mathcal{B}(X)} \leq M$ for all $0 \leq s \leq 1$. Writing any $t \geq 0$ as $t = s + n$ with $n \in \mathbb{N}$ and $s \in [0, 1]$,

$$\|T(t)\|_{\mathcal{B}(X)} \leq \|T(s)\|_{\mathcal{B}(X)}\, \|T(1)\|^n_{\mathcal{B}(X)} \leq M^{n+1} = Me^{n\log M} \leq Me^{wt}$$

holds for $\omega := \log M$ and $t \geq 0$. ■

Definition 8.2.3 *If lemma 8.2.2 holds for $\omega = 0$ and $M = 1$, the semigroup is called contractive. It means that $\|T(t)\|_{\mathcal{B}(X)} \leq 1$ for all $t \geq 0$.*

Example 8.2.4 *Let $\mathcal{H}$ be a Hilbert space, $A \in \mathcal{B}(\mathcal{H}) := X$. It can be easily shown that the series*

$$e^{tA} := \sum_{n=0}^{\infty} \frac{1}{n!}(tA)^n$$

converges and that $T(t) := e^{tA}$ defines a C^0-group. From the triangle inequality, we deduce that

$$\|T(t)\|_{\mathcal{B}(X)} \leq e^{t\|A\|_X},$$

and therefore lemma 8.2.2 holds for $M = 1$ and $\omega = \|A\|_X \in \mathbb{R}$.

Remark 8.2.5 (Abstract Cauchy problem) *In Example 8.2.4, we have been able to define a C^0-group from a bounded operator. This group satisfies*

$$\begin{cases} \dot{T}(t) = AT(t) \text{ for all } t \geq 0 \\ T(0) = \mathbf{1}_X. \end{cases} \tag{8.1}$$

The main topic studied in this article is the existence and properties of such an A for a general C^0-semigroup $(T(t))_{t\geq 0}$ by using the abstract Cauchy problem (8.1).

Definition 8.2.6 *A C^0-semigroup $(T(t))_{t\geq 0}$ is called uniformly continuous if the map*

$$\begin{array}{rcl} \mathbb{R}^+ & \longrightarrow & X \\ t & \longmapsto & \|T(t)\|_{\mathcal{B}(X)} \end{array}$$

is continuous.

Proposition 8.2.7 *Let $(T(t))_{t\geq 0}$ be a uniformly continuous semigroup. Then, there exists a bounded operator A on X such that $T(t) = e^{tA}$ for all $t \geq 0$.*

For more details, see [41, Theorem 2.12]. Within this article, we focus our study on the general case of strong continuity. In this case, the existence of such a bounded operator A requires a deeper study of operator semigroups, see 8.2.5. We start by defining the generator of a C^0-semigroup.

Definition 8.2.8 (Generator) *The generator $A : D(A) \subseteq X \to X$ of a C^0-semigroup $(T(t))_{t\geq 0}$ is the operator*

$$Ax := \dot{\xi}_x(0) = \lim_{h\downarrow 0} \frac{1}{h}(T(h)x - x)$$

with domain

$$D(A) = \left\{ x \in X : \lim_{h\downarrow 0} \frac{1}{h}(T(h)x - x) \text{ exists} \right\}.$$

Note that the orbit map ξ_x is differentiable on $\mathbb{R}^+$ if and only if it is right-differentiable at $t = 0$. Indeed, the derivative of $\xi_x(t)$ at any t depends only on the derivative at $t = 0$ in the following way:

$$\dot{\xi}_x(t) = T(t)\dot{\xi}_x(0). \tag{8.2}$$

The following lemma summarizes some (basic) properties of the generator. They will be used throughout the proofs of the upcoming results.

Lemma 8.2.9 *Let $(A, D(A))$ be the generator of a C^0- semigroup $(T(t))_{t\geq 0}$. Then:*

(i) $A : D(A) \to X$ is a linear operator.

(ii) If $x \in D(A)$, then $T(t)x \in D(A)$ and, for all $t \geq 0$:

$$\frac{d}{dt}T(t)x = T(t)Ax = AT(t)x.$$

(iii) For all $t \geq 0$ and $x \in X$,

$$\int_0^t T(s)xds \in D(A).$$

(iv) For all $t \geq 0$,

$$T(t)x - x = \begin{cases} A\int_0^t T(s)xds & \text{if } x \in X, \\ \int_0^t T(s)Axds & \text{if } x \in D(A). \end{cases}$$

Proof:

(i) From definition 8.2.8, it is clear that A is a linear operator and that $D(A)$ is a linear subspace of X.

(ii) Let $x \in D(A)$. Since $T(t)$ is bounded for all $t \geq 0$,

$$T(t)Ax = T(t)\lim_{h\downarrow 0}\frac{1}{h}(T(h)x - x) = \lim_{h\downarrow 0}\frac{1}{h}(T(h)T(t)x - T(t)x) = AT(t)x$$

with $\frac{d}{dt}(T(t)x) := T(t)\lim_{h\downarrow 0}\frac{1}{h}(T(h)x - x)$, and hence

$$T(t)Ax = \frac{d}{dt}(T(t)x) = AT(t)x.$$

(iii) For all $t \geq 0$ and $x \in X$,

$$\begin{aligned} \lim_{h\downarrow 0}\frac{1}{h}\left(T(h)\int_0^t T(s)xds - \int_0^t T(s)xds\right) &= \lim_{h\downarrow 0}\left(\frac{1}{h}\int_0^t T(s+h)xds - \frac{1}{h}\int_0^t T(s)xds\right) \\ &= \lim_{h\downarrow 0}\left(\frac{1}{h}\int_t^{t+h} T(s)xds - \frac{1}{h}\int_0^h T(s)xds\right) \\ &= T(t)x - x. \end{aligned}$$

(Note that the last limit holds from the Fundamental Theorem of Calculus).

(iv) Note that from what we have just seen, for any $x \in X$,

$$Tx - x = \lim_{h\downarrow 0} \frac{1}{h}\left(T(h)\int_0^t T(s)xds - \int_0^t T(s)xds\right) = A\int_0^t T(s)xds.$$

Moreover, if $x \in D(A)$, note that

$$\left\| T(s)\frac{T(h)x - x}{h} - T(s)Ax \right\|_X \le \|T(s)\|_{\mathcal{B}(X)} \left\| \frac{T(h)x - x}{h} - Ax \right\|_X.$$

Hence, on $s \in [0, t]$, for any $t \ge 0$ we have the following uniform comvergence:

$$T(s)\frac{T(h)x - x}{h} \xrightarrow[h\downarrow 0]{u} T(s)Ax.$$

Therefore, for any $x \in D(A)$,

$$\lim_{h\downarrow 0} \frac{1}{h}(T(h) - \mathbf{1}_X)\int_0^t T(s)xds = \int_0^t T(s)\lim_{h\downarrow 0}\left(\frac{1}{h}T(h) - \mathbf{1}_X\right)xds = \int_0^t T(s)Axds.$$

This concludes the proof

■

The following theorems give us further properties of the generator.

Theorem 8.2.1 *The generator A of a C^0-semigroup $(T(t))_{t\ge 0}$ is closed, densely defined and it determines the semigroup uniquely.*

Proof: Let us prove A is closed. Suppose there is a sequence $(x_n)_{n\in\mathbb{N}} \subset D(A)$ such that $x_n \to x \in X$, for $n \to \infty$. Suppose that $Ax_n \to y \in X$, for $n \to \infty$. It suffices by the characterization of closed operators to show that $x \in D(A)$ and $Ax = y$. Since $x_n \in D(A)$, for $t > 0$, one has (see Lemma 8.2.9):

$$T(t)x_n - x_n = \int_0^t T(s)Ax_n \mathrm{d}s \tag{8.3}$$

Now let's see that $\int_0^t T(s)Ax_n\mathrm{d}s$ converges to $\int_0^t T(s)y\mathrm{d}s$ as $n \to \infty$. By strng continuity, the map $s \in [0, t] \mapsto T(s)y$ is integrable over $[0, t]$. By the triangular inequality of integrals

$$\left\| \int_0^t T(s)Ax_n\mathrm{d}s - \int_0^t T(s)y \right\|_X = \left\| \int_0^t T(s)(Ax_n - y)\mathrm{d}s \right\|_X \le \int_0^t \|T(s)(Ax_n - y)\|_X \mathrm{d}s$$

$$\le \int_0^t \|T(s)\|_{\mathcal{B}(X)} \|Ax_n - y\| \mathrm{d}s \le \left(\int_0^t Me^{\omega t}\right) \|Ax_n - y\|_X$$

Here we have used lemmas 8.2.9 and 8.2.2. The sequence of inequalities follows from triangular inequality for integrals, boundedness of $T(s)$ by strong continuity and the exponential growth bound. Since $\int_0^t Me^{\omega t}$ is a bounded number $\forall t \geq 0$ and Ax_n converges to y, we deduce that indeed $\lim_{n\to\infty} \int_0^t T(s)Ax_n \mathrm{d}s = \int_0^t T(s)y\mathrm{d}s$. But strong continuity of the semigroups yields that $\lim_{n\to\infty} T(t)x_n - x_n = T(t)x - x$. By uniqueness of limits we conclude from equation (8.3) that

$$T(t)x - x = \int_0^t T(s)y\mathrm{d}s \quad \forall t \geq 0$$

When t is taken to be positive we have:

$$\frac{1}{t}(T(t)x - x) = \frac{1}{t}\int_0^t T(s)y\mathrm{d}s$$

When t approaches zero we are simply taking the derivative of $T(t)x$ at $t = 0$. That limit exists by the fundamental theorem of vector calculus (the integrand $T(s)y$ is continuous). This implies that

$$Ax = \frac{\mathrm{d}}{\mathrm{d}t}(T(t)x)\,|_{t=0} = T(0)y = y$$

This means that $Ax = y$ is well-defined, thus $x \in D(A)$. Hence A is closed.

To see that A is densely defined, let us consider $x \in X$. By Lemma 8.2.9,

$$\int_0^t T(s)x\mathrm{d}s \in D(A), \quad \text{for all } t > 0.$$

Moreover, since T is strongly continuous, taking the limit $t \to 0$ is possible again by the fundamental theorem of vector calculus. This yields

$$\lim_{t\to 0}\frac{1}{t}\int_0^t T(s)x\mathrm{d}s = T(0)x = x$$

Thus $D(A)$ is a dense subspace of X.
Finally, to prove that A determines the semigroup uniquely we suppose there is another strongly continuous semigroup $(S(t))_{t\geq 0}$ such that its generator is $A : D(A) \to X$. Let $x \in D(A)$ and $t \geq 0$ be fixed. To see that they are the same semigroup, we define the auxiliary function:

$$s \in [0,t] \mapsto \psi_{t,x}(s) = T(t-s)S(s)x.$$

We will differentiate this at $s \in [0,t]$. Consider the quotient:

$$\frac{1}{h}(\psi_{t,x}(s+h) - \psi_{t,x}(s)) = \frac{1}{h}(T(t-s-h)S(s+h)x - T(t-s)S(s)x) =$$

$$= \left[T(t-s-h)\frac{1}{h}(S(s+h)x - S(s)x)\right] + \left[\frac{1}{h}(T(t-s-h) - T(t-s))S(s)x\right]$$

The second term converges to $-AT(t-s)S(s)x$ as $h \to 0$, since $S(s)x \in D(A)$ by lemma 8.2.9. The minus sign comes from the chain rule: $-A$ is the generator of $s \mapsto T(t-s)$.

We will prove that the first term converges to $T(t-s)AS(s)x$ when $h \to 0$. We will consider $h \in [0, t-s]$.

$$\left\| T(t-s-h)\frac{1}{h}(S(s+h)x - S(s)x) - T(t-s)AS(s)x \right\|_X \leq$$

$$\leq \left\| T(t-s-h)\frac{1}{h}(S(s+h)x - S(s)x) - T(t-s-h)AS(s)x \right\|_X + \|T(t-s-h)AS(s)x - T(t-s)S(s)x\|_X$$

$$\leq \|T(t-s-h)\|_{\mathcal{B}(X)} \left\| \frac{1}{h}(S(s+h)x - S(s)x) - AS(s)x \right\|_X + \|T(t-s-h)[AS(s)x] - T(t-s)[AS(s)x]\|_X$$

The first term goes to zero as $h \to 0$ because $\|T(t-s-h)\|_{\mathcal{B}(X)}$ is exponentially bounded by $Me^{\omega(t-s-h)}$ (see lemma 8.2.2) and the second term vanishes due to strong continuity. Therefore we have proven that:

$$\frac{\mathrm{d}}{\mathrm{d}s}\psi_{t,x}(s) = T(t-s)AS(s)x + -AT(t-s)S(s)x$$

Since semigroups and generators commute (here $-A$ is the generator of $T(t-s)$), we conclude that:

$$\frac{\mathrm{d}}{\mathrm{d}s}\psi_{t,x}(s) = 0 \ \ \forall s \in [0,t]$$

Therefore $\psi_{t,x}$ is constant:

$$T(t)x = \psi_{t,x}(0) = \psi_{t,x}(t) = S(t)x$$

Hence $T(t)$ and $S(t)$ agree on $D(A)$, which is dense on X. Then they agree on all X. ■

Now, we are going to see some definitions and properties to prove the Hille Yosida theorem.

Definition 8.2.10 *Let $\lambda \in C^*$ and A a closed linear operator. The* ***resolvent set*** *of A is defined by*

$$\rho(A) := \{\lambda \in C^* : (\lambda \mathbf{1}_X - A) \text{ is bijective}\}$$

and $R(\lambda, A) := (\lambda \mathbf{1}_X - A)^{-1}$ is called the resolvent map of A.

Remark 8.2.11 *Let $(T(t))_{t\geq 0}$ be a semigroup. For $\mu \in C^*$ and $\alpha > 0$, we define the rescaled semigroup $(S(t))_{t\geq 0}$ by*

$$S(t) = e^{\mu t}T(\alpha t), \quad t \geq 0.$$

Note that if $(A, D(A))$ is the generator of $(T(t))_{t\geq 0}$, $(\alpha\mathbf{1}_X, D(\mu\mathbf{1}_X + \alpha A))$ is the generator of $(S(t))_{t\geq 0}$ and the resolvent map is $R(\lambda, \mu\mathbf{1}_X + \alpha A) = \frac{1}{\alpha}R(\frac{\lambda}{\alpha} - \frac{\mu}{\alpha}, A)$ for $\lambda \in \rho(\mu\mathbf{1}_X + \alpha A)$

Theorem 8.2.2 *Let $(T(t))_{t\geq 0}$ be a strongly continuos semigroup on the Banach space X and $(A, D(A))$ its generator. If $\lambda \in C^*$ such that*

$$R(\lambda) := \int_0^{+\infty} e^{-\lambda s} T(s)x ds \quad \forall x \in X, \quad \textit{is well-defined},$$

then $\lambda \in \rho(A)$ and $R(\lambda) = R(\lambda, A)$.

Proof: By without loss of generality, rescaling the semigroup, we can assume that $\lambda = 0$. Note that the existence of such a λ is ensured by Lemma 8.2.2. Therefore, one needs to show that $0 \in \rho(A)$. In particular, we will show that $R(0) = R(0, A) = (-A)^{-1}$. For all $x \in X$, $h > 0$

$$\frac{T(h) - \mathbf{1}_X}{h} R(0)x = \frac{T(h) - \mathbf{1}_X}{h} \int_0^{+\infty} T(s)x ds = \frac{1}{h} \int_0^{+\infty} T(s+h)x ds - \frac{1}{h} \int_0^{+\infty} T(s)x ds =$$

$$= \frac{1}{h} \int_h^{+\infty} T(s)x ds - \frac{1}{h} \int_0^{+\infty} T(s)x ds = -\frac{1}{h} \int_0^h T(s)x ds.$$

Moreover,

$$\lim_{h \to 0} \left(\frac{1}{h} \int_0^h T(s)x ds \right) = x.$$

Thus, $R(0)x \in D(A)$ and $A\, R(0) = -\mathbf{1}_X$. Furthermore, if $x \in D(A)$ we have that

$$\lim_{t \to +\infty} \int_0^t T(s)x ds = R(0)x.$$

And, by Lemma 8.2.9,

$$\lim_{t \to +\infty} A \int_0^t T(s)x ds = \lim_{t \to +\infty} \int_0^t T(s)Ax ds = R(0)Ax.$$

finally, by theorem 8.2.1, we deduce that

$$R(0)Ax = AR(0)x = -x, \text{ for } x \in D(A).$$

This concludes the proof. ■

Corollary 8.2.12 *Let $(T(t))_{t\geq 0}$ be a strongly continous semigroup such that*

$$||T(t)||_{\mathcal{B}(X)} \leq M e^{\omega t} \quad \omega \in \mathbb{R}, \quad M \geq 1.$$

If $\lambda \in \mathbb{C}$ and $\omega < Re(\lambda)$, then

$$||R(\lambda, A)||_{\mathcal{B}(X)} \leq \frac{M}{Re(\lambda) - \omega}.$$

Proof: For $t, t' \geq 0$,

$$\left\| \int_{t'}^{t} e^{-\lambda s} T(s) ds \right\|_{\mathcal{B}(X)} \leq M \int_{t'}^{t} e^{(\omega - \mathrm{Re}\lambda)s} ds.$$

By the Cauchy criterium, for $\omega < \mathrm{Re}(\lambda)$,

$$\int_0^\infty e^{(\omega - \mathrm{Re}\lambda)s} ds \quad \text{exists.}$$

Therefore, by Theorem 8.2.2, $\lambda \in \rho(A)$ and

$$R(\lambda, A) = \int_0^\infty e^{-\lambda s} T(s) ds.$$

Obviously,

$$\|R(\lambda, A)\|_{\mathcal{B}(X)} \leq M \int_0^\infty e^{(\omega - \mathrm{Re}(\lambda))s} ds = \frac{M}{\mathrm{Re}(\lambda) - \omega}.$$

This concludes the proof. ■

Hille-Yosida Generation Theorem

So far, we have given necessary properties for an operator to be a generator of a strongly continuous semigroup on X. In particular, for a strongly continuous contraction semigroup $(T(t))_{t\geq 0}$, we know by Theorem 8.2.1 that its generator $(A, D(A))$ is closed and densely defined. Moreover, because of Corollary 8.2.12 and Definition 8.2.3, for every $\lambda \in \mathbb{C}$ such that $\mathrm{Re}\lambda > 0$, $\lambda \in \rho(A)$ and

$$\|R(\lambda, A)\|_{\mathcal{B}(X)} \leq \frac{1}{Re\lambda}.$$

Now we are going to show that these conditions are sufficient for contraction semigroup. First we recall a result that will be useful in the sequel.

Lemma 8.2.13 ([41], Ch. I, §1, Proposition 1.3) *Let $(T(t))_{t\geq 0}$ be a semigroup. If there exists a dense subset $D \subset X$, $\delta > 0$ and $M \geq 1$ such that:*

(i) $\|T(t)\|_{\mathcal{B}(X)} \leq M, \quad \forall t \in [0, \delta]$

(ii) $\lim_{t\downarrow 0} T(t)x = x, \quad \forall x \in D$

then $(T(t))_{t\geq 0}$ is a strongly continuous semigroup.

Theorem 8.2.3 (Hille-Yosida, 1948) *Let $(A, D(A))$ be a linear operator on a Banach space X. The following statements are equivalent:*

(i) $(A, D(A))$ *generates a strongly continuous contraction semigroup.*

(ii) $(A, D(A))$ *is closed, densely defined, and* $\forall \lambda > 0$, $\lambda \in \rho(A)$ *and* $\|\lambda R(\lambda, A)\|_{\mathcal{B}(X)} \leq 1$.

(iii) $(A, D(A))$ *is closed, densely defined, and* $\forall \lambda \in \mathbb{C}$ *with* $Re\lambda > 0$, $\lambda \in \rho(A)$ *and* $\|R(\lambda, A)\|_{\mathcal{B}(X)} \leq \frac{1}{Re\lambda}$.

Proof: Note that (*i*) yields (*iii*) by an application of Corollary 8.2.12. Moreover, (*ii*) is a straightforward conclusion of (*iii*). Thus, it remains to prove (*ii*) $\Rightarrow$ (*i*).

To that purpose, we define the *Yosida approximants*

$$A_n := nAR(n, A) = n^2 R(n, A) - nI, \; n \in \mathbb{N}$$

Note that, for each $n \in \mathbb{N}$,

$$\|A_n\|_{\mathcal{B}(X)} \leq n \, \|nR(n, A)\|_{\mathcal{B}(X)} + n \leq 2n.$$

Moreover, since

$$(n - A)(m - A) = (m - A)(n - A)$$

one has

$$R(n, A)R(m, A) = R(m, A)R(n, A) \quad \text{and} \quad [A_n, A_m] = 0.$$

These properties imply that the semigroups $(T_n(t))_{t\geq 0}$ given by $T_n(t) := e^{tA_n}$, $t \geq 0$ are uniformly continuous, and mutually commute.

Because of the fact that $A_n x = nAR(n, A)x = n^2 R(n, A)x - nI$ converges to Ax for $x \in D(A)$ (see [41], Ch. II, §3, Proposition 3.4), we can anticipate the following properties.

(a) $T(t)x := \lim_{n\to\infty} T_n(t)x$ exists for each $x \in X$.

(b) $(T(t))_{t\geq 0}$ is a C^0- contraction semigroup on X.

(c) This semigroup has generator $(A, D(A))$.

In order to prove (*a*), we observe that $(T_n(t))_{t\geq 0}$ is a contraction semigroup for each $n \in \mathbb{N}$:

$$\|T_n(t)\|_{\mathcal{B}(X)} \leq e^{-nt} e^{\|n^2 R(n,A))\|_{\mathcal{B}(X)} t} \leq e^{-nt} e^{nt} = 1 \text{ for } t \geq 0, \quad \text{by assumption (ii).} \tag{8.4}$$

Now by using the mutual commutativity of the semigroups $(T_n(t))_{t\geq 0}$ for all $n \in \mathbb{N}$ and the vector-valued version of the fundamental theorem of calculus, for $x \in D(A)$, $t \geq 0$, $m, n \in \mathbb{N}$,

$$T_n(t)x - T_m(t)x = \int_0^t \frac{d}{ds}(T_m(t-s)T_n(s)x)ds = \int_0^t T_m(t-s)T_n(s)(A_n x - A_m x)ds.$$

By using the triangle inequality and (8.4), we obtain that

$$\|T_n(t)x - T_m(t)x\|_{\mathcal{B}(X)} \leq t\|A_n x - A_m x\|_{\mathcal{B}(X)}. \tag{8.5}$$

For $x \in D(A)$, since $(A_n x)_{n\in\mathbb{N}}$ is a Cauchy sequence, $(T_n(t)x)_{n\in\mathbb{N}}$ is a Cauchy sequence, i.e, $(T_n(t)x)_{n\in\mathbb{N}}$ converges to some $T(t)x$. Now let $x \in X$. Since $D(A)$ is dense in X, one has

$$\forall \varepsilon > 0, \exists y \in D(A) : \|x - y\|_X < \varepsilon.$$

Therefore,

$$\|T_n(t)x - T_m(t)x\|_{\mathcal{B}(X)} \leq \|T_n(t)(x-y)\|_{\mathcal{B}(X)} + \|T_n(t)y - T_m(t)y\|_{\mathcal{B}(X)} + \|T_m(t)(y-x)\|_{\mathcal{B}(X)}.$$

Observe that the right side of the inequality is arbitrarily small as n, m goes to ∞ because $(T_n(t))_{n\in\mathbb{N}}$ is a Cauchy sequence. Hence, $(T_n(t)(x))_{n\in N}$ is a Cauchy sequence, for all $t \geq 0$ and $x \in X$. Therefore, it converges to some $T(t)x$, for all $x \in X$.

In (b), one needs to prove that the family of operators defines above is a strongly continuous contraction semigroup. First, observe that

$$x = \lim_{n\to\infty} T_n(0)x = T(0)x.$$

Hence,

$$T(0) = \mathbf{1}_X.$$

Moreover, for $t, s \geq 0$,

$$T(t+s)x = \lim_{n\to\infty} T_n(t+s)x = \lim_{n\to\infty} T_n(t)T_n(s)x. \tag{8.6}$$

Furthermore, for $t, s \geq 0$,

$$T_n(t)T_n(s)x = T_n(t)T(s)x + T_n(t)(T_n(s) - T(s))x.$$

Finally, observe that

$$\lim_{n\to\infty} \|T_n(t)(T_n(s) - T(s))x\|_X = 0$$

and

$$\lim_{n\to\infty} T_n(t)T(s)x = T(t)T(s)x.$$

By (8.6) we thus deduce the semigroup property.

To prove that the family $(T(t))_{t\geq 0}$ is strongly continuous, note that, by (8.5), for all $x \in D(A)$, $T(s)x$ is actually the uniform limit of $T_n(s)x$ on the interval $[0, t]$. The maps $s \in [0, t] \mapsto T_n(s)x$ are continuous. Hence, the uniform limit $s \in [0, t] \mapsto T(s)x$ is also continuous. From (8.4), $\|T(t)\| \leq 1$ for all $t \geq 0$. So by using lemma 8.2.13 with $D = D(A)$ we conclude the family is strongly continuous.

To finish the proof, it remains to show that the generator of $(T(t))_{t\geq 0}$, namely $(B, D(B))$, is $(A, D(A))$. Fix any $x \in D(A)$. The orbit map

$$\xi_x : t \in [0, t_0] \mapsto \xi_x(t) = T(t)x$$

is the uniform limit of

$$\xi_x^n : t \in [0, t_0] \mapsto \xi_x^n(x) = T_n(t)x.$$

Also, their derivatives

$$\frac{d}{dt}\xi_x^n : t \in [0, t_0] \mapsto T_n(t)A_n x$$

converge uniformly to

$$\eta_x : t \mapsto T(t)Ax.$$

Indeed, for $t \in [0, t_0]$

$$\|T_n(t)A_n x - T(t)Ax\|_{\mathcal{B}(X)} \leq \|T_n(t)(A_n x - Ax)\|_{\mathcal{B}(X)} + \|(T_n(t) - T(t))Ax\|_{\mathcal{B}(X)}$$

and the right hand side vanishes as n goes to ∞ uniformly with respect to $t \in [0, t_0]$. Since

$$\xi_x^n(t) = x + \int_0^t \frac{d}{ds}\xi_x^n(s)ds = x + \int_0^t T_n(s)A_n x ds,$$

by taking $n \to \infty$, we have

$$\xi_x(t) = \lim_{n\to\infty} \xi_x^n(t) = x + \int_0^t T(s)Axds = x + \int_0^t \eta_x(s)ds.$$

Thus, ξ_x is differentiable with $\frac{d}{dt}\xi_x(t)|_{t=0} = \eta(0) = Ax$, i.e. $D(A) \subseteq D(B)$ and $Ax = Bx$, for $x \in D(A)$.

Now let $\lambda > 0$. By hypothesis, $\lambda \in \rho(A)$. Since $(B, D(B))$ is the generator of the contraction semigroup $(T(t))_{t\geq 0}$, $\lambda \in \rho(B)$. Thus, both $(\lambda - A)$ and $(\lambda - B)$, possibly unbounded, admit a bounded inverse operator mapping the whole space onto the domain of the generator. Then, for every $y \in D(B)$, we get that

$$(\lambda - B)y = \mathbf{1}_X(\lambda - B)y = (\lambda - A)\underbrace{R(\lambda, A)(\lambda - B)y}_{\in D(A)}. \tag{8.7}$$

Moreover, since A and B agree on $D(A)$

$$(\lambda - B)y = (\lambda - B)R(\lambda, A)(\lambda - B)y. \tag{8.8}$$

By applying $R(\lambda, B)$ on both sides we get

$$y = R(\lambda, A)(\lambda - B)y \in D(A). \tag{8.9}$$

This implies that $D(B) \subset D(A)$, thus $(A, D(A)) = (B, D(B))$. This concludes the proof. ■

A generalization of Hille-Yosida theorem was set in 1952 by Feller, Miyadera & Phillips. Its proof relies on the generation theorem proved by Hille and Yosida, which can be applied after a rescaling argument and a renormalization of the space.

Theorem 8.2.4 (General Generation Theorem, Feller-Miyadera-Phillips, 1952) *Let $(A, D(A))$ be a linear operator on a Banach space X and let $\omega \in \mathbb{R}$, $M \geq 1$ be constants. Then, the following properties are equivalent.*

(i) $(A, D(A))$ *generates a* C^0*-semigroup* $(T(t))_{t\geq 0}$ *satisfying*

$$\forall t \geq 0, \quad \|T(t)\| \leq Me^{wt}. \tag{8.10}$$

(ii) $(A, D(A))$ *is closed, densely defined, and for all* $\lambda > \omega$, $\lambda \in \rho(A)$ *and*

$$\forall n \in \mathbb{N} \quad \|\,[(\lambda - \omega)R(\lambda, A)]^n\,\| \leq M. \tag{8.11}$$

(iii) $(A, D(A))$ *is closed, densely defined, and for all* $\lambda \in \mathbb{C}$ *such that* $Re\lambda > \omega$, $\lambda \in \rho(A)$ *and*

$$\forall n \in \mathbb{N} \quad \|R(\lambda, A)^n\| \leq \frac{M}{(Re\lambda - \omega)^n}. \tag{8.12}$$

Proof: (*i*) implying (*iii*) is proven in [41, Corollary 1.11]. We shall omit this proof for a matter of space. Then (*iii*) implies immediately (*ii*). Thus, we will detail the fact that (*ii*) implies (*i*).

It has already been seen that, if A generates $(T(t))_{t\geq 0}$, $A - \omega$ generates $(e^{-wt}T(t))_{t\geq 0}$. Furthermore, the resolvent satisfies

$$R(\lambda, A - \omega) = R(\lambda + \omega, A).$$

Hence, for any $\lambda > 0$, $\lambda \in \rho(A - \omega)$. One can assume without loss of generality that $\omega = 0$. Therefore, by hypothesis

$$\forall n \in \mathbb{N} \quad \|\lambda^n R(\lambda, A)^n\| \leq M. \tag{8.13}$$

Note that throughout the rest of the proof, as it has already been defined previously, $R(\lambda, A)$ is denoted by $R(\lambda)$.

Now, we define, for any $\mu > 0$, the following norm on X

$$\|x\|_\mu := \sup_{n\geq 0} \|\mu^n R(\mu)^n x\|_X, \tag{8.14}$$

which is equivalent to $\|\cdot\|_X$. In fact, the estimate $\|x\|_\mu \leq M\|x\|_X$ follows from Equation (8.13). By taking $n = 0$ in (8.14) we get the equivalence of norms:

$$\forall x \in X, \quad \|x\|_X \leq \|x\|_\mu \leq M\|x\|_X. \tag{8.15}$$

Moreover,

$$\|\mu R(\mu)x\|_\mu = \sup_{n\geq 1} \|\mu^n R(\mu)^n x\|_X \leq \sup_{n\geq 0} \|\mu^n R(\mu)^n x\|_X = \|x\|_\mu. \tag{8.16}$$

Let $0 < \lambda \leq \mu$ and fix some $x \in X$. Observe that, for $R(\lambda)x \in D(A)$ and $R(\mu)(\mu - A)$ acting as the identity on $D(A)$,

$$R(\lambda)x = R(\mu)(\mu - A)R(\lambda)x = R(\mu)(\mu - \lambda)R(\lambda)x + R(\mu)(\lambda - A)R(\lambda)x = R(\mu)(x + (\mu - \lambda)R(\lambda)x). \tag{8.17}$$

By the triangle inequality on μ-norms,

$$\|R(\lambda)x\|_\mu \leq \|R(\mu)x\|_\mu + \|(\mu - \lambda)R(\mu)R(\lambda)x\|_\mu, \tag{8.18}$$

and by using Equation (8.16) we obtain that

$$\|\lambda R(\lambda)x\|_\mu \leq \|x\|_\mu. \tag{8.19}$$

Together with the norm equivalence in (8.15) this inequality implies

$$\|\lambda^n R(\lambda)^n x\|_X \leq \|\lambda^n R(\lambda)^n x\|_\mu \leq \|x\|_\mu. \tag{8.20}$$

By considering the supremum over n of the left hand side, we obtain the following property of the μ-norms:

$$\forall x \in X, \quad \|x\|_\lambda \leq \|x\|_\mu \text{ for } 0 < \lambda \leq \mu. \tag{8.21}$$

Because of Equation (8.15),

$$|||x||| := \sup_{\mu>0} \|x\|_\mu \tag{8.22}$$

is well-defined and actually defines another norm on X. Because of the equivalence relation of the μ-norms, the norm $|||\cdot|||$ satisfies

$$\forall x \in X, \quad \|x\|_X \leq |||x||| \leq M\|x\|_X. \tag{8.23}$$

One concludes that $|||\lambda R(\lambda)||| \leq 1$. Thus, $(A, D(A))$ satisfies the hypothesis of Theorem 8.2.3 and generates a $|||\cdot|||$-contraction semigroup $(T(t))_{t\geq 0}$ in the Banach space $(X, |||\cdot|||)$. It follows from the equivalence of the $|||\cdot|||$-norm and the previous norm established in Equation (8.23) that, for every $t \geq 0$,

$$\|T(t)\|_{\mathcal{B}(X)} \leq M.$$

This concludes the proof. ■

Hilbert space generation theorems

In this section we give a proof of Stone's Theorem based on Hendrik Kuiper's lecture notes, which can be found in [44, Section 3.3]. Let $\mathcal{H}$ be a Hilbert space. First of all, given a strongly continuous semigroup $(T(t))_{t\geq 0} \subset \mathcal{B}(\mathcal{H})$ one shall define its *adjoint semigroup* as $(T(t)^*)_{t\geq 0}$. Note that, since $T(t)^*T(s)^* = (T(s)T(t))^* = T(t+s)^*$, for $t, s \geq 0$, the adjoint semigroup is well-defined.

Proposition 8.2.14 *Let $(A, D(A))$ be the generator of the C^0-semigroup $(T(t))_{t\geq 0}$ acting on a Hilbert space $\mathcal{H}$. Then, its adjoint semigroup is strongly continuous with generator $(A^*, D(A^*))$.*

Proof: For $(T(t))_{t\geq 0}$ being strongly continuous there exist $M \geq 0$, $\omega \in \mathbb{R}$ such that the growth bound $\|T(t)\|_{\mathcal{B}(\mathcal{H})} \leq Me^{\omega t}$ holds. Since $\|T(t)^*\|_{\mathcal{B}(\mathcal{H})} = \|T(t)\|_{\mathcal{B}(\mathcal{H})}$, the adjoint semigroup satisfies the same inequality. Let $x \in D(A)$ be a normalised vector and $z \in D(A^*)$. Then, by the properties stated in Lemma 8.2.9

$$\langle x, T(t)^*z - z\rangle = \langle T(t)x - x, z\rangle = \int_0^t \langle AT(\tau)x, z\rangle d\tau = \int_0^t \langle x, T(\tau)^*A^*z\rangle d\tau. \tag{8.24}$$

Thus, by Cauchy-Schwarz and triangle inequalities [1]

$$|\langle x, T(t)^*z - z\rangle| \leq \int_0^t \|T(\tau)^*\|_{\mathcal{B}(\mathcal{H})}\|A^*z\|_{\mathcal{H}} d\tau \leq Mte^{\omega t}\|A^*z\|_{\mathcal{H}}. \tag{8.25}$$

Since $D(A)$ is dense in $\mathcal{H}$, it follows from above that $\|T(t)^*z - z\|_{\mathcal{H}} \leq Mte^{\omega t}\|A^*z\|_{\mathcal{H}}$. Therefore, $\lim_{t\downarrow 0} T(t)^*z = z$ for every $z \in D(A)$. Moreover, for $t_0 > 0$ and $t \in [0, t_0]$, $\|T(t)^*\| \leq Me^{\omega t_0}$ ($M = 1$, $\omega = 0$ in the contraction case). By Lemma 8.2.13, the adjoint semigroup is strongly continuous.

Suppose that $(B, D(B))$ is the generator of the adjoint semigroup. let $x \in D(A)$ and $y \in D(B)$. Observe that

$$\langle Ax, y\rangle = \lim_{t\downarrow 0} \frac{1}{t}\langle T(t)x - x, y\rangle = \lim_{t\downarrow 0} \frac{1}{t}\langle x, T(t)^*y - y\rangle = \langle x, By\rangle. \tag{8.26}$$

Therefore, $D(B) \subset D(A^*)$, by definition of $D(A^*)$. Moreover, since $D(A)$ is dense, (8.24) implies that, for $z \in D(A^*)$,

$$T(t)^*z - z = \int_0^t T(\tau)^*A^*z d\tau. \tag{8.27}$$

Hence

$$Bz = \lim_{h\downarrow 0} \frac{1}{h}(T(h)^*z - z) = \lim_{h\downarrow 0} \frac{1}{h}\int_0^t T(\tau)^*A^*z d\tau = A^*z \tag{8.28}$$

holds and $D(A^*) \subset D(B)$ and $A^* = B$. ■

A (possibly unbounded) operator A acting on a Hilbert space is said to be *skew-adjoint* whenever $A^* = -A$. The next theorem, due to Stone, deals with generators satisfying this property. The proof given in [44, Theorem 3.3.5] has been modified in order to apply Hille-Yosida contraction generation theorem. As we will see in the next section, the generators of evolution groups in quantum mechanics are skew-adjoint.

Theorem 8.2.5 (Stone, 1932) *Let $(A, D(A))$ be an operator acting on a Hilbert space. Then, $(A, D(A))$ generates a unitary C^0–group $(U(t))_{t\in\mathbb{R}}$ if and only if A is skew-adjoint.*

[1] Note that the exponential term in the right-hand-side of Equation (8.25) should be omitted in the contraction case.

Proof: If $(U(t))_{t\in\mathbb{R}}$ is a unitary C^0–group, then A^* is the generator for $U(t)^* = U(t)^{-1} = U(-t)$ as it was shown in the previous theorem. Given any $x \in D(A)$,

$$\lim_{h\downarrow 0} \frac{1}{h}(U(h)^* x - x) = \lim_{h\downarrow 0} \frac{1}{h}(U(-h)x - x) = -Ax, \tag{8.29}$$

so $x \in D(A^*)$. Since the left hand side equals A^*x, $D(A) \subset D(A^*)$ and $-A$ agrees with A^* along its domain. One could repeat the same argument for arbitrary $x \in D(A^*)$, obtaining $D(A^*) \subset D(A)$. Therefore, $D(A) = D(A^*)$ and A is skew-adjoint.

On the other hand, note that if $(A, D(A))$ is skew-adjoint, then $(iA, D(A))$ is self-adjoint. Thus, both $(A, D(A))$ and $(A^*, D(A^*)) = (-A, D(A))$ have a purely imaginary spectrum (lying on $i\mathbb{R}$). It follows that

$$\|\lambda R(\lambda, A)\|_{\mathcal{B}(\mathcal{H})} \leq \sup_{\mu\in i\mathbb{R}} \frac{\lambda}{|\lambda + \mu|} \leq 1. \tag{8.30}$$

The same calculation is satisfied by $-A$ trivially. Therefore, because of Hille-Yosida generation theorem in the contraction case, $(A, D(A))$, respectively $(-A, D(A))$, is the generator of the semigroup $(U(t)^+)_{t\geq 0}$, respectively $(U(t)^-)_{t\geq 0}$.

Now, we proceed to show that $(U(t))_{t\in\mathbb{R}}$ defined by

$$U(t) = \begin{cases} U(t)^+ & t \geq 0 \\ U(-t)^- & t < 0 \end{cases}, \tag{8.31}$$

is a unitary C^0-group. Indeed, the strong continuity follows after its definition. It is only left to prove that $(U(t))_{t\in\mathbb{R}}$, with composition as a product, is a group.

We proceed to show that $U(t)$, $U(-t)$ are inverse elements with $U(0) = \mathbf{1}_{\mathcal{H}}$ as identity element. To this end, fix any $x \in D(A)$. For $t = 0$, $U(0)^+U(0)^-x = \mathbf{1}_{\mathcal{H}}x = x$. Then, for $t > 0$, because of the derivative properties of C^0-semigroups and the skew-adjointness of $(A, D(A))$

$$\frac{d}{dt}U(t)^+U(t)^-x = \left[U(t)^+AU(t)^- + U(t)^+A^*U(t)^-\right]x = 0. \tag{8.32}$$

Thus, for $t > 0$, $U(t)^+U(t)^-x = x$, and $D(A)$ is dense in $\mathcal{H}$, so $U(t)U(-t) = \mathbf{1}_{\mathcal{H}}$.

In order to prove that $(U(t))_{t\in\mathbb{R}}$ is closed under composition, fix any $t, s > 0$. $U(t)U(s) = U(t+s)$ and $U(-t)U(-s) = U(-t-s)$ for $(U(t)^+)_{t\geq 0}$ and $(U(t)^-)_{t\geq 0}$ being semigroups. If $t < s$, $U(t)U(-s) = U(t)U(-t)U(t-s) = U(t-s)$ and the $t > s$ case follows similarly. Since composition is associative, $(U(t))_{t\in\mathbb{R}}$ is a group and the proof is over. ■

Back to quantum mechanics

In the setting of quantum mechanics, as it was explained in the introduction, the space of all possible states of the system is modeled by a Hilbert space $\mathcal{H}$. The energy of the system, described by the self-adjoint Hamiltonian H, determines the evolution of the system via *Schrödinger's equation*:

$$\begin{cases} i\partial_t \psi(t,x) = H\psi(t,x), \\ \psi(0,x) = \psi_0(x) \in \mathcal{H}. \end{cases} \tag{8.33}$$

As one can see in (1.2), the solution of the above system has the form $\psi(t,x) = U(t)\psi_0(x)$, where $U(t) \in \mathcal{B}(\mathcal{H})$ for $t \in \mathbb{R}$. Again, by (1.2), $U(t)$ satisfies

$$\begin{cases} \partial_t U(t) = -iHU(t), \\ U(0) = \mathbf{1}_{\mathcal{H}}. \end{cases} \tag{8.34}$$

For H being a self-adjoint operator, H is densely defined, and so it is for $-iH$. Thus, Stone Theorem assures that $-iH$ will generate a strongly continuous unitary group $(U(t))_{t\in\mathbb{R}}$ satisfying the functional equation in (8.34).

In terms of the wavefunction interpretation, it is needed that the evolution semigroup preserves the norm of the original state ψ_0. Otherwise, there would be an undesirable loss (or gain) of probability if, for example,

$$\|\psi_t\|_{\mathcal{H}} < \|\psi_0\|_{\mathcal{H}} = 1. \tag{8.35}$$

Stone Theorem ensures this will not occur. Since the evolution operator is unitary, it is guaranteed that in $\mathcal{H}$

$$\|\psi_t\|_{\mathcal{H}} = \|U(t)\psi_0\|_{\mathcal{H}} = \|\psi_0\|_{\mathcal{H}} = 1. \tag{8.36}$$

In terms of the Heisenberg picture introduced in Section 1.1, the time evolution of an observable B in a system determined by the Hamiltonian H is given by the action of a strongly continuous group $\{\tau_t\}_{t\in\mathbb{R}}$ on $\mathcal{B}(\mathcal{H})$. This time evolution is defined by $\tau_t(B) := \mathrm{e}^{itH}B\mathrm{e}^{-itH}$, for $t \in \mathbb{R}$ and $B \in \mathcal{B}(\mathcal{H})$. These operators satisfy the equation

$$\begin{cases} \partial\tau_t = \tau_t \circ \delta = \delta \circ \tau_t \\ \tau_0 = \mathbf{1}_{\mathcal{B}(\mathcal{H})} \end{cases} \tag{8.37}$$

where $\delta : D(\delta) \subset \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ is a symmetric derivation defined on a dense subset $D(\delta)$ of $\mathcal{B}(\mathcal{H})$. It can be proved that these symmetric derivations satisfy the hypothesis of the Hille-Yosida Generation Theorem. Therefore, they are the generators of the C^0-group $\{\tau_t\}_{t\in\mathbb{R}}$ and determine uniquely the evolution of the physical system.

In fact, the δ operators described above belong to the class of *dissipative operators*, which are contained in the core of the Lumer-Phillips Generation Theorem (see [41, Theorem 3.15]). This theorem allows to adapt the Hille-Yosida Generation Theorem to dissipative operators, in a similar way as the Stone Theorem, which ajusts our main theorem to self-adjoint operators.

Ny hany hafatro dia ny hoe matokia.
Andrianabela Rakotobe.

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