

The Schrödinger equation and Uncertainty Principles

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PhD Thesis

Basque Centre for Applied Mathematics BCAM Bilbao, July 2020

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by

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Memoria realizada bajo la dirección del catedrático de Análisis Dr. D. Luis Vega González, para optar al grado de Doctor en Ciencias, Sección de Matemáticas, por la Universidad del País Vasco - Euskal Herriko Unibertsitatea.

No theorist in his right mind would have invented quantum mechanics unless forced by data.

Abstract

The main task of this thesis is the analysis of the initial data u_0 of Schrödinger's initial value problem in order to determine certain properties of its dynamical evolution.

First we consider the elliptic Schrödinger problem in its perturbative form. The idea is to find lower bounds for the solution giving conditions at time t = 0 together with a size condition on the potential. After analyzing the elliptic case we give a similar result for the hyperbolic Schrödinger operator.

Next we focus on the free particle case, this is, the case where no potential is involved. The goal here is to quantify the L^2 norm of the solution in a space-time cylinder. Following the same idea as before we want to find conditions at time t = 0 to ensure this. To carry out this task we define the Σ_{δ} space where δ is a parameter on the interval (0, 1]. We see that if u_0 belongs in this space then so does its evolution in time and use this fact to give lower bounds for the L^2 norm of the solution. For $\delta = 1$ we give a different approach and make use of the Virial Theorem. We will see that this case has particular properties.

Finally we study dynamical uncertainty principles derived from the previous study. The key point will be to write the solution as $u = \rho e^{i\theta}$, where ρ and θ are real functions. Thus we give uncertainty principles in terms of these functions and find explicit expressions for them so that u becomes a minimizer of the problem.

Agradecimientos

Antes que nada me gustará dedicar este trabajo a mi amama que desgraciadamente falleció el mismo mes en que empezaba el doctorado. Ella siempre me dijo que llegaría donde me propusiese y estoy seguro de que allá donde esté se siente feliz y orgullosa. Eskerrik asko amama.

Hace casi seis años terminé mi máster en la Universidad de Copenhague y tocaba decidir qué hacer a continuación. Para un chaval de 24 años con gran pasión por las matemáticas y la idea de poder ser docente universitario parecía que un doctorado era la opción ideal. Y me lancé a la piscina. Resultó ser la piscina de *Schrödinger*, tenía agua y no al mismo tiempo.

No voy a mentir y decir que ha sido un camino de rosas porque la verdad es que se ha parecido más a la travesía desde *Hobbiton* hasta *Mordor* y a mí no me gusta *El señor de los anillos*. No obstante, e igual que le sucedió a *Frodo*, me he sentido bien acompañado a lo largo del viaje y quiero aprovechar estas líneas para dar las gracias ya que sin estas personas ni siquiera habría salido de *La Comarca*.

En primer lugar quiero dar las gracias a mi director de tesis Luis Vega. Creo que ni él mismo es consciente de las veces que me ha salvado de caer por un precipicio. Siempre que las fuerzas flaqueaban ahí estaba Luis con palabras de ánimo y confianza. Confianza que ni yo mismo tengo sobre mí. Por eso y por la infinita paciencia que este hombre ha tenido conmigo, que ha sido impagable. Eskerrik asko.

Siguiendo un poco la jerarquía laboral, me gustaría hacer especial mención sobre el colega Aingeru *Skywalker* que me ha tendido una mano siempre que lo he necesitado y ha sacado tiempo para recibirme tanto en la Universidad como virtualmente. A todas las personas que me acompañaron en BCAM, desde *internships* hasta miembros del *staff*, a todos y cada uno mil millones de gracias. Y entre toda esta gente quiero destacar a Miguel, que ha amenizado cada uno de mis trámites burocráticos, a Gabriela, que sólo con sonreír ya me alegraba los días, a Marco, por ser mi compañero fiel, y a Imanol, por ser tan payaso como yo.

Más allá del ámbito laboral, en primer lugar viene mi familia. Es imposible expresar aquí todo el agradecimiento que tengo hacia ellos, no solo por haberme apoyado siempre incondicionalmente sino porque toda mi formación tanto profesional como personal se la debo a ellos. Asko maite zaituztet.

Quiero a continuación agradecer a todos mis amigos. Sería imposible nombrarlos de uno en uno si no esto se extendería más incluso que la propia tesis así que optaré por un agradecimiento geográfico. A todos mis amigos de Gernika, Durango, Markina, Mungia, Portugalete, Getxo, Bilbo, Donosti, Gasteiz, Iruña, Madrid, Barcelona y Valencia. Este viaje hubiera sido muy aburrido sin vosotros, mila esker guztiagatik.

A mis compañeros de la Universidad de Mondragón que me acogieron con los brazos abiertos desde el primer momento y hacen que mi trabajo sea fácil. En especial quiero dar las gracias a Iván Gallego porque fue mi mentor cuando empecé y siempre me ha animado mucho con la tesis y también a Josune Urien por ser una inspiración constante de mujer.

Para finalizar me gustaría también dar las gracias a Rafa, Julio, Martin y Fred, que hicieron de mi estancia en Estrasburgo un periodo maravilloso. Os deseo toda la suerte del mundo en vuestras vidas y ya sabéis que mi casa es vuestra casa.

Regarding my stay in Strasbourg I would also like to thank professor Raphael Cote for inviting me to their University and for letting me be a part of their group. And also a special mention to professor Nalini Anantharaman who helped me greatly progress on my thesis.

And last but not the least, I would like to thank professors J. Marzuola and F. Linares for revising my thesis and for their suggestions that certainly helped improve the work.

Durante la realización de la tesis he contado con el apoyo económico de las siguientes fuentes:

- Programa predoctoral del Departamento de Educación, Política Lingüistica y Cultura del Gobierno Vasco.
- Ayudas para estancias en centros distintos al de aplicación del Programa Predoctoral de Formación de Personal Investigador
- ERCEA Advanced Grant 2014 669689 HADE.
- MEIC projects MTM2014-53850-P y SEV-2013-0323.
- Programa BERC del Gobierno Vasco.

Resumen

Una mirada a la mecánica cuántica

La mecánica cuántica es la parte de la física que estudia el movimiento de las partículas muy pequeñas o microobjetos. Esta nueva rama surgió de la necesidad de dar respuesta a fenómenos físicos para los que la mecánica clásica no tenía respuesta, como por ejemplo la imposibilidad de dar explicaciones ante conceptos como la radiación del cuerpo negro. En esta dirección, las primeras propuestas llegaron a principios del siglo XX de la mano del físico alemán *Max Planck*.

Sin embargo, no fue hasta mediados de la década de 1920 cuando los fundamentos de la mecánica cuántica fueron establecidos. Uno de los pioneros en el campo fue el físico francés *Louis de Broglie*, quien descubrió la naturaleza corpuscularondulatoria de los objetos físicos. Ejemplo de ello es la luz que en la totalidad del siglo XIX se creía que tenía propiedades exclusivamente ondulatorias pero más adelante pudo demostrarse que se comportaba también como partícula.

Tras *de Broglie*, aparecieron ilustres científicos como el físico austríaco *Erwin Schrödinger*, que es precisamente quien da nombre a esta tesis, o el matemático y físico alemán *Max Born*. Éste último fue quien propuso en un artículo publicado en 1926 el carácter probabilístico de la teoría.

Hemos mencionado dos de los elementos fundamentales de la teoría cuántica que son por un lado la dualidad onda-partícula de los objetos, como la interpretación probabilística que se esconde tras ella. Estos conceptos pueden entenderse muy bien mediante el experimento de la doble rendija realizado por el científico inglés *Thomas Young* cuyo objetivo era discernir la naturaleza corpuscular u ondulatoria de la luz. En la segunda mitad del siglo XX el mismo experimento fue realizado con electrones de la mano del físico alemán *Clauss Jönsson*. Más tarde en 1989 un grupo liderado por el físico japonés *Akira Tonomura* llevó a cabo el mismo experimento que describimos a continuación.

El experimento consta de un panel con dos rendijas separadas a una distancia a y una pantalla colocada a distancia d del panel, que es donde colisionarán los electrones. De esta forma se disparan las partículas, preparadas de la misma forma,

y se registran las colisiones en la pantalla. Se puede observar que cuando una de las rendijas está tapada el registro de colisiones no muestra ninguna interferencia. En este caso, se genera una patrón semejante a una Gaussiana donde la mayor densidad de colisiones se produce en frente de la rendija abierta. Sin embargo, cuando los electrones tienen ambas vías abiertas el registro de las colisiones es algo más complejo.

Supongamos ahora que ambas rendijas están abiertas. Si disparamos un electrón cada vez veremos que éste impacta en un único punto de la pantalla y su posición queda totalmente registrada y así sucede con cada uno de los electrones que disparamos. La clave está en que cada electrón genera un único punto y no se dispersa como cabría esperar de un comportamiento ondulatorio. Sin embargo, la posición en la que una única partícula colisiona es completamente aleatoria y al disparar gran cantidad de éstas se genera un patrón de interferencia.

Lo sorprendente no es la variación de puntos en los que los electrones colisionan sino el claro patrón de interferencia que deja a relucir cuáles son las zonas con mayor número de colisiones y cuáles las zonas en las que apenas llega ninguno como se puede apreciar en las siguientes imágenes:



Figure 1: Imagen tomada de [14], p. 13, correspondiente al experimento de la doble rendija llevado a cabo en 1989 por el grupo liderado por Akira Tonomura.

La primera imagen se corresponde con la distribución de las colisiones de 150 electrones y no se aprecia ningún tipo de patrón. Sin embargo, la última imagen

corresponde a la distribución de 160.000 electrones y en este caso sí es posible detectarlo.

Es precisamente este patrón de interferencia el que hace referencia al carácter ondulatorio de los electrones. Por supuesto, si disparamos un único electrón no seremos capaces de predecir en qué punto de la pantalla colisionará pero podemos estimar la probabilidad de que lo haga en un punto concreto utilizando una función que caracterice el patrón que ya hemos mencionado. Esta función será precisamente la *función de onda* que describe a nuestro sistema de electrones.

Esta función de onda toma como argumento valores $x \in \mathbb{R}^n$, que debemos entender como posibles puntos en los que la partícula puede encontrarse, y cuya evolución en tiempo vendrá determinada por la *ecuación de Schrödinger*. Cabe recalcar que esta función de onda no representa el comportamiento de una sola partícula sino que establece el comportamiento estadístico de un sistema (o sucesión) de partículas al que nos referiremos como **sistema cuántico**.

A pesar de ser una sobre-simplificación podemos entender la naturaleza corpuscular-ondulatoria de un sistema cuántico de la siguiente forma: una única partícula del sistema se comportará precisamente como tal, pero una sucesión de éstas dará lugar a un comportamiento ondulatorio.

En esta tesis nos referiremos a la función de onda que caracteriza el sistema cuántico como u = u(x, t) donde como ya hemos dicho $x \in \mathbb{R}^n$ y t será la variable temporal que determine su evolución dinámica. La función u lleva así codificada toda la información referente al sistema. En particular, la cantidad $|u(x, t)|^2$ define la densidad de probabilidad relacionada a la posición. Tiene por tanto sentido asumir que se verifica lo siguiente,

$$\int_{\mathbb{R}^n} |u(x,t)|^2 dx = 1,$$

para todo tiempo t. Es decir, que la probabilidad de encontrar una partícula en algún punto del espacio es absoluta.

Queda claro que a niveles cuánticos no podemos hablar de certidumbre a la hora de hacer mediciones, cosa que era relativamente sencillo en la mecánica clásica, ya que en este caso las partículas quedan unívocamente determinadas por los valores de posición y momento en un instante t. A lo máximo a lo que podemos aspirar ahora es a conocer las probabilidades de estas magnitudes. Hasta ahora hemos hablado únicamente de la posición de una partícula pero podemos hablar de otras magnitudes físicas como el momento de un sistema cuántico.

En mecánica cuántica las cantidades físicas (posición, momento, energía,...) se representan mediante operadores definidos en un espacio de Hilbert \mathcal{H} . Nos

interesa además que estos operadores sean autoadjuntos. Recordemos primero que el producto interior entre dos vectores cualesquiera en un espacio de Hilbert \mathcal{H} se define como

$$\langle u, v \rangle = \int_{\mathbb{R}^n} u \bar{v} dx, \quad \forall u, v \in \mathcal{H}(\mathbb{R}^n).$$

Definición. Sea el operador lineal S definido en un espacio de Hilbert \mathcal{H} . Definimos el operador adjunto de S, al que llamaremos S^* como el operador que verifica

$$\langle u, Sv \rangle = \langle S^*u, v \rangle,$$

para cualquier vector $v \in \mathcal{D}(S)$ y $u \in \mathcal{D}(S^*)$.

Definición. Se dice que un operador lineal S es hermítico si

$$Su = S^*u, \quad \forall u \in \mathcal{D}(S)$$

si además de esto $\mathcal{D}(S) = \mathcal{D}(S^*)$ podremos afirmar estrictamente que $S = S^*$ y en este caso diremos que el operador S es **autoadjunto**.

Definición. De la misma forma, diremos que un operador lineal A es anti hermítico si

$$Au = -A^*u, \quad \forall u \in \mathcal{D}(A).$$

Supongamos una partícula moviéndose en la recta real \mathbb{R} . Sabemos por la teoría de probabilidades de que la *esperanza matemática* de la posición viene dada por

$$\int_{\mathbb{R}} x |u(x,t)|^2 dx,$$

para cualquier tiempo t fijado. Si definimos S = x como el operador posición vemos que podemos escribir la integral de arriba mediante el producto interior del espacio de Hilbert correspondiente,

$$\langle Su, u \rangle.$$

Una de las principales ideas de la teoría cuántica es precisamente la posibilidad de representar las *esperanzas matemáticas* de diferentes magnitudes físicas usando operadores y el producto interior tal y como hemos hecho para la posición de la partícula.

Otra de las magnitudes con las que trabajaremos en esta tesis es el momento. Esta magnitud se representa mediante el operador $S = -i\partial_x$ en dimensión 1 o $S = -i\nabla$ si hablamos de dimensiones mayores. Una de las particularidades del momento de un sistema cuántico es que su información está codificada en el espacio frecuencial de tal forma que el momento de una partícula puntual sea $p = \hbar \xi$ donde \hbar es la constante de Planck y ξ es la variable frecuencial. Esta observación es importante ya que sugiere una relación directa entre nuestra función de onda y su transformada de Fourier. Es más, veremos que esta relación implica la imposibilidad de medir de manera simultánea la posición y el momento de una partícula. Esta propiedad se denomina *Principio de incertidumbre* y es una de las características más importantes dentro de la teoría cuántica.

Definimos la transformada de Fourier de una función f como

$$\hat{f}(\xi) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-ix\cdot\xi} f(x) dx,$$

donde $x \cdot \xi = x_1 \xi_1 + \ldots + x_n \xi_n$ es el producto escalar.

De esta forma tiene sentido construir u como superposición de funciones definidas en el espacio frecuencial usando la transformada inversa de Fourier

$$u(x,t) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{ix \cdot \xi} \hat{u}(\xi,t) d\xi.$$

La ecuación de Schrödinger

Queda claro que existen grandes diferencias entre la mecánica clásica y la cuántica. Hemos mencionado que para el primer caso un sistema físico queda completamente definido si conocemos su posición x y su momento lineal p en un instante t_0 . Podemos incluso definir la dinámica del sistema en el tiempo y hablar de trayectorias, cosa que no es posible en el esquema cuántico.

Sin embargo, no deja de ser lógico suponer que el sistema evolucionará en el tiempo y con él la función de onda que hemos denominado como u. De esta forma diremos que para un instante t el estado estará descrito por $u_t(x) = u(x,t)$ donde el tiempo no juega más que el papel de un parámetro. ¿Cómo podemos caracterizar esta evolución en el tiempo si no podemos hablar de trayectorias de manera explícita?

De esto se encarga la ecuación presentada por el físico austríaco *Erwin* Schrödinger en 1926

$$i\hbar\frac{\partial}{\partial t}u(x,t) = Hu(x,t),$$

denominada como ecuación de Schrödinger dependiente del tiempo donde \hbar es la constante de Planck y H es el operador Hamiltoniano que caracteriza la energía total del sistema.

La ecuación de Schrödinger presentada arriba es la formulación física que podemos encontrar en la literatura. Nosotros trabajaremos en un contexto matemático y plantearemos el problema de valores iniciales de Schrödinger de la siguiente forma a lo largo de esta tesis,

$$\begin{cases} \partial_t u(x,t) = i(\Delta u(x,t) + V(x,t)u(x,t)), & x \in \mathbb{R}^n, t \in \mathbb{R} \\ u(x,0) = u_0(x), \end{cases}$$
(1)

donde V será un potencial y Δ es el laplaciano que definimos como

$$\Delta = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}.$$

Nos referiremos al caso particular en que no haya ningún potencial actuando sobre nuestro sistema como caso de la partícula libre. Además cuando trabajemos en este contexto introduciremos un factor 1/2 para simplificar cálculos de forma que la ecuación quede de la siguiente forma

$$\partial_t u = \frac{i}{2} \Delta u. \tag{2}$$

Para el caso de la partícula libre podemos calcular la solución de manera explícita usando las propiedades de la transformada de Fourier. Así la ecuación (2) se transforma en

$$\partial_t \hat{u}(\xi, t) = -\frac{i}{2} |\xi|^2 \hat{u}(\xi, t),$$

y resolvemos

$$\hat{u}(\xi, t) = \hat{u}_0(x)e^{-\frac{i}{2}t|\xi|^2}$$

Usando ahora la fórmula de inversión para la transformada de Fourier podemos recuperar nuestra solución u de (2) de forma que obtenemos

$$u(x,t) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-ix\cdot\xi} \hat{u}(\xi,t) d\xi = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-ix\cdot\xi} e^{-\frac{i}{2}t|\xi|^2} \hat{u}_0(\xi) d\xi$$

O de manera más compacta como

$$u(x,t) = e^{it\Delta}u_0(x) = \frac{1}{(2\pi i t)^{n/2}} \int_{\mathbb{R}^n} e^{i\frac{|x-\xi|^2}{2t}} u_0(\xi) d\xi,$$
(3)

donde $i^{1/2} = e^{i\pi/4}$ cuando t > 0. Si consideramos t < 0 tendríamos que tomar su conjugada, $i^{1/2} = e^{-i\pi/4}$.

Esta representación de la solución nos dice además que la ecuación de Schrödinger se sitúa en el marco de las ecuaciones dispersivas.

Otra de las características de la solución del caso de la partícula libre es que si u es solución del problema (2) también lo serán sus derivadas espaciales siempre que éstas existan.

Principios de incertidumbre

Hemos mencionado que en el contexto de la mecánica cuántica, cuando hablamos de la posición y el momento de un sistema cuántico, nos es imposible medir con precisión ambas magnitudes al mismo tiempo. Este fenómeno se conoce como el principio de incertidumbre y fue enunciado en [47] por el físico alemán *Werner Karl Heisenberg* en 1927.

Matemáticamente el principio de incertidumbre de Heisenberg se formula de la siguiente forma,

$$\frac{2}{n} \left(\int_{\mathbb{R}^n} |xf(x)|^2 dx \right)^{1/2} \left(\int_{\mathbb{R}^n} |\nabla f(x)|^2 dx \right)^{1/2} \ge \int_{\mathbb{R}^n} |f(x)|^2 dx.$$
(4)

También podemos obtener (4) como caso particular de un principio de incertidumbre abstracto como vemos a continuación

Sea \mathcal{H} un espacio de Hilbert y S y A operadores hermítico y anti-hermítico respectivamente, es decir, para una función apropiada ψ ,

$$\langle S\psi,\psi\rangle = \langle\psi,S\psi\rangle, \qquad \langle A\psi,\psi\rangle = -\langle\psi,A\psi\rangle.$$

Observamos entonces que para el operador S + A y para $\psi \in \mathcal{D}(S) \cap \mathcal{D}(A)$ tenemos,

$$0 \leq ||(A+S)\psi||^{2} = \langle S\psi, S\psi \rangle + \langle A\psi, A\psi \rangle + \langle S\psi, A\psi \rangle + \langle A\psi, S\psi \rangle$$
$$= \langle S\psi, S\psi \rangle + \langle A\psi, A\psi \rangle + 2Re\langle S\psi, A\psi \rangle$$
$$= \langle S\psi, S\psi \rangle + \langle A\psi, A\psi \rangle + \langle (SA - AS)\psi, \psi \rangle.$$

Por lo tanto,

$$-\langle (SA - AS)\psi, \psi \rangle \le ||S\psi||^2 + ||A\psi||^2.$$
(5)

Si hacemos un cálculo similar y cambiamos el operador anti-hermítico ${\cal A}$ por $-{\cal A}$ obtenemos,

$$\langle (SA - AS)\psi, \psi \rangle \le ||S\psi||^2 + ||A\psi||^2, \tag{6}$$

y combinando (5) y (6) vemos que

$$|\langle (SA - AS)\psi, \psi \rangle| \le ||S\psi||^2 + ||A\psi||^2.$$
 (7)

Sea $\lambda > 0$ y definimos

$$\tilde{A} = \lambda A, \qquad \tilde{S} = \frac{1}{\lambda}S.$$

Si ahora metemos \tilde{A} y \tilde{S} en (6) obtenemos

$$|\langle (SA - AS)\psi, \psi \rangle| \le \frac{1}{\lambda^2} ||S\psi||^2 + \lambda^2 ||A\psi||^2.$$
(8)

Ahora bien, como hemos escogido un λ de forma arbitraria, tomamos $\lambda^2 = \frac{||S\psi||}{||A\psi||}$ de tal manera que la ecuación (8) se transforma en

$$|\langle (SA - AS)\psi, \psi \rangle| \le 2||S\psi|| \ ||A\psi||. \tag{9}$$

La desigualdad (9) es precisamente el principio de incertidumbre. Por otra parte, la desigualdad se convierte en igualdad si y solo si

$$(S+A)\psi = 0.$$

Una de las aplicaciones del Principio de incertidumbre sería tomar $\mathcal{H} = L^2(\mathbb{R})$ y considerar los operadores

$$S\psi = x\psi, \qquad A\psi = \frac{d}{dx}\psi = \psi'.$$

De esta forma obtendríamos el principio de incertidumbre de Heisenberg que hemos mencionado anteriormente. Si calculamos ahora el conmutador de estos operadores obtenemos,

$$(SA - AS)\psi = \left(x\frac{d}{dx} - \frac{d}{dx}x\right)\psi = x\psi' - (x\psi)'$$
$$= x\psi' - \psi - x\psi' = -\psi.$$

Observamos que por (9),

$$-\langle (SA - AS)\psi, \psi \rangle = \langle \psi, \psi \rangle \le 2\left(\int |x\psi|^2\right)^{1/2} \left(\int |\psi'|^2\right)^{1/2}.$$
 (10)

Tendremos igualdad solamente si $\psi' = -x\psi$, es decir, si la suma de los operadores es idénticamente 0 como hemos mencionado arriba. Si resolvemos la ecuación diferencial ordinaria correspondiente obtenemos $\psi_0 = Ce^{-x^2/2}$ que es precisamente la función que nos proporciona la igualdad en (10), lo cual convierte a ψ_0 en un minimizante del problema. Veremos que las Gaussianas surgen de manera natural cuando tratamos de encontrar minimizantes de principios de incertidumbre. Por otro lado se cumple

$$0 = \left\langle (A+S)\psi, (A+S)\psi \right\rangle = \left\langle (S-A)(S+A)\psi, \psi \right\rangle = \left\langle \left(S^2 - A^2 + SA - AS\right)\psi, \psi \right\rangle,$$

de tal forma que ψ_0 verifica la siguiente ecuación diferencial,

$$-\frac{d^2}{dx^2}\psi_0(x) + x^2\psi_0(x) = \psi_0(x).$$

Por tanto vemos que ψ_0 resuelve el problema del oscilador armónico y además vemos que es una autofunción del problema para el autovalor asociado $\lambda = 1$.

Podemos replantear el principio de incertidumbre en términos de una función y su transformada de Fourier. Recordemos uno de los resultados fundamentales dentro de la teoría de Fourier, la denominada *igualdad de Plancherel*. Este resultado nos dice que la norma L^2 de una función y su transformada son iguales

$$\int_{\mathbb{R}^n} |f(x)|^2 dx = \int_{\mathbb{R}^n} |\hat{f}(\xi)|^2 d\xi.$$

Usando esta igualdad junto con propiedades de la transformada podemos ahora reescribir (4) como

$$\frac{2}{n} \left(\int_{\mathbb{R}^n} |xf(x)|^2 dx \right)^{1/2} \left(\int_{\mathbb{R}^n} |\xi \hat{f}(\xi)|^2 d\xi \right)^{1/2} \ge \int_{\mathbb{R}^n} |f(x)|^2 dx.$$

Además la igualdad se alcanzará cuando las integrales del lado izquierdo sean proporcionales. Así vemos que las funciones que minimizarán el problema son funciones cuya transformada de Fourier son ellas mismas siendo ésta una de las propiedades de las Gaussianas.

Queda claro que las Gaussianas juegan un papel importante en el marco de los principios de incertidumbre y la velocidad con la que decaen una función y su transformada de Fourier. Siguiendo esta línea hablamos del principio de incertidumbre de Hardy [11], que fue probado por el matemático británico Godfrey H. Hardy en 1933. Concretamente, este resultado nos dice que

$$|f(x)| \le Ce^{-\alpha|x|^2}, \quad |\hat{f}(\xi)| \le Ce^{-\beta|x|^2}, \quad \alpha\beta > \frac{1}{4} \Rightarrow f \equiv 0.$$
(11)

Además si $\alpha\beta = 1/4$ se tiene que la función f debe ser una Gaussiana, $f(x) = Ce^{-\alpha|x|^2}$. La demostración de este resultado usa técnicas de variable compleja y no profundizaremos más aquí; no obstante el lector puede referirse a [34], [35] y [36] para obtener más detalles. El principio de incertidumbre de Hardy ha sido objeto de estudio durante largo tiempo y ha sido extendido a dimensiones mayores e incluso ha sido planteado en contextos más generales por autores como Bonami-Demange-Jaming, Cowling-Price, Hörmander y Sitaram-Sundari-Thangavelu en [37], [38], [39], [40], [41], [42], [43] entre otros.

Podemos relacionar el principio de incertidumbre de Hardy con la solución de Schrödinger de una manera sencilla. Si escribimos (3) como

$$u(x,t) = \frac{1}{(2\pi i t)^{n/2}} e^{i\frac{|x|^2}{2t}} \left(\widehat{e^{i\frac{|\cdot|^2}{2t}} u_0} \right) \left(\frac{x}{t}\right).$$
(12)

Observamos que la solución del problema viene representada como la transformada de Fourier del dato inicial debidamente modulada. Esto nos indica que dar condiciones de tamaño de la solución u a dos tiempos es equivalente a dar condiciones de tamaño sobre la solución u y la transformada del dato inicial. Utilizando esta premisa se puede utilizar el principio de incertidumbre de Hardy para dar un resultado cualitativo sobre u,

Si
$$e^{\frac{|x|^2}{\beta^2}}u_0(x), e^{\frac{|x|^2}{\alpha^2}}e^{it\Delta}u_0(x) \in L^2(\mathbb{R}^n) \text{ y } \alpha\beta \leq 4t, \text{ entonces } u_0 \equiv 0.$$
 (13)

En una serie de artículos de L. Escauriaza, C.E. Kenig, G. Ponce y L. Vega entre los que encontramos [4], [6], [10], se dan resultados de continuación única de carácter cualitativo motivados por el principio de incertidumbre de Hardy. El objetivo de estos trabajos es enunciar resultados del mismo tipo pero usando argumentos de variable real y en contextos perturbativos, es decir, considerando que haya un potencial V actuando sobre el sistema cuántico. Para ello se buscan condiciones a dos tiempos y se establece únicamente una condición de tamaño sobre el potencial, en concreto

$$\lim_{R \to +\infty} \int_0^1 \|V(t)\|_{L^{\infty}(\mathbb{R}^d \setminus B_R)} dt = 0,$$

donde B_R es la bola de radio R, para concluir que la única solución del problema es $u \equiv 0$. Además se aplican estos resultados sobre soluciones del problema no-lineal

$$i\partial_t u + \Delta u = \pm |u|^2 u,$$

para dar resultados de unicidad.

Una de las técnicas utilizadas en estos trabajos son las estimaciones de Carleman que permiten trabajar en contextos perturbativos. En particular, en [4] se utiliza la siguiente desigualdad de Carleman

$$\frac{\sigma^{3/2}}{c_n R^2} \left\| e^{\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} g \right\|_2 \le \left\| e^{\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} \left(i\partial_t + \Delta \right) g \right\|_2, \tag{14}$$

para probar que la única solución que puede decaer más rápido que $e^{-a|x|^2}$ para a suficientemente grande, es la solución trivial. En (14) c_n es una constante que

$$\left\{ (x,t) : \left| \frac{x}{R} + \varphi e_1 \right| \ge 1 \right\}.$$

Hasta ahora hemos hablado de principios de incertidumbre relacionados con el decaimiento (gaussiano) de las funciones y sus correspondientes transformadas de Fourier. Otra versión de éstos nos dice que una función y su transformada no pueden estar simultáneamente localizadas en el espacio. Esto se traduce en que si una función no-nula f es de soporte compacto su transformada no puede satisfacer una condición de la forma $\hat{f}(\xi) = \mathcal{O}(e^{-\epsilon|\xi|})$ para cualquier $\epsilon > 0$.

Esto se debe a que $\hat{f}(\xi) = \mathcal{O}(e^{-\epsilon|\xi|})$ implica que f se puede extender de manera analítica a la banda $\{z \in \mathbb{C}^n : |Im(z)| < \epsilon\}$. Estos resultados se denominan principios de incertidumbre de tipo Paley-Wiener en honor al matemático británico *Raymond Paley* y el filósofo y matemático americano *Norbert Wiener*. Estos principios de incertidumbre permiten caracterizar funciones de soporte compacto en función de las propiedades analíticas de su transformada.

En otro artículo de C.E. Kenig, G. Ponce y L. Vega [7], como en los arriba mencionados, se buscan condiciones a dos tiempos para concluir que $u \equiv 0$. Estas condiciones serán del tipo Paley-Wiener. La estrategia utilizada en este artículo es una combinación de la desigualdad de Carleman junto con transformaciones de Appell. Éstas nos permiten generar una familia de soluciones de (1) mediante dilataciones en las variables espacio-tiempo. Definiendo la función g de la desigualdad de Carleman de manera adecuada, las transformaciones de Appell nos permiten ajustar las regiones de integración en función de los parámetros de dilatación.

En el **capítulo 1** de la tesis utilizaremos esta misma estrategia para buscar resultados cuantitativos para la solución de (1). Además, queremos reducir las hipótesis iniciales sobre la solución, de dos tiempos a uno único. La idea así es buscar condiciones sobre el dato inicial que nos aseguren que la evolución dinámica del sistema se preserva. El punto de partida es un resultado utilizado en [4], concretamente el Teorema 3.1. En éste se dan cotas por debajo para la solución udel problema

$$i\partial_t u + \Delta u + V u = 0, \quad t \in [0, 1], \quad x \in \mathbb{R}^n,$$

y su gradiente en una región $\{R - 1 \le |x| \le R\} \times [0, 1]$ donde el tamaño de Rdepende de la norma u en el espacio correspondiente y el tamaño del potencial V. Una de las hipótesis del teorema asume que en un cilindro espacio-tiempo alrededor del origen y para tiempos $t \sim 1/2$ la norma L^2 de la solución está controlada por debajo, es decir,

$$\int_{1/2-1/8}^{1/2+1/8} \int_{|x|<1} |u|^2(x,t) dx dt \ge 1.$$
(15)

De esta forma se concluye que para un c = c(n),

$$\delta(R) \equiv \left(\int_0^1 \int_{R-1 < |x| < R} \left(|u|^2 + |\nabla_x u|^2 \right) (x, t) dx dt \right)^{1/2} \ge c e^{-cR^2}, \qquad (16)$$

es decir, que el decaimiento de la solución u tiene que ser al menos Gaussiano. El resultado principal del capítulo 1 queda recogido en 1.4.1. La demostración de este teorema sigue el mismo esquema que la del teorema 3.1 de [4] con la diferencia de que introducimos las transformaciones de Appell como ya hemos mencionado. Gracias a éstas conseguimos reducir la integral en tiempo a costa de modificar la región de la variable espacial. En particular, nos permite estimar la norma \mathcal{H}^1 de la solución en tiempos pequeños y en una región particular del espacio.

Veremos además que esta región es dinámica en el sentido de que varía con respecto a ciertos parámetros espacio temporales. Estos parámetros nos permiten de hecho dar propiedades de unicidad para las soluciones del problema. Estos resultados están enunciados en los teoremas 1.4.2 y 1.4.3.

Otra de las ventajas del teorema 1.4.1 es que admite potenciales V complejos dependientes del tiempo lo cual nos permite extender los resultados a casos no lineales siempre y cuando el problema esté bien definido y tengamos los recursos necesarios para desarrollarlo. De esta forma podemos tratar problemas del tipo

$$\partial_t u = i \left(\Delta u + f \left(|u|^2 \right) u \right),$$

para f real y f(0) = f'(0) = 0.

Veremos además que el uso de la desigualdad de Carleman da lugar a la aparición del término del gradiente de la solución. Es natural preguntarse si es posible quitar este término de manera que se pueda concluir un resultado de observabilidad como en [45], [46]. El problema está en que nuestra ecuación de Schrödinger admite potenciales que dependen de las variables espacio-tiempo. En [1] se presenta un resultado de observabilidad en $\mathbb{T}^n := (\mathbb{R}/2\pi\mathbb{Z})^n$ para potenciales que no dependan del tiempo. Siguiendo la misma línea, en [45] se da un resultado de observabilidad con condiciones periódicas para el problema

$$i\partial_t u(t,z) = (-\Delta + V(z))u(t,z), \quad z \in \mathbb{T}^2$$

donde $\mathbb{T}^2 := \mathbb{R}^2 / A\mathbb{Z} \times B\mathbb{Z}, A, B \in \mathbb{R} \setminus \{0\}$ y el potencial $V \in \mathcal{C}(\mathbb{T}^2)$ es real.

Terminaremos el primer capítulo analizando precisamente el caso de la solución periódica. Veremos cómo cambia el teorema 1.4.1 para este tipo de soluciones y cómo afecta a la región en la que observamos tanto a la solución como a su gradiente. En el **capítulo 2**, siguiendo una sugerencia del profesor J. Marzuola, extendemos los resultados obtenidos previamente al problema hiperbólico de Schrödinger, es decir,

$$\begin{cases} \partial_t u = i(\Delta_1 - \Delta_2 + V(x, t))u\\ u(x, 0) = u_0(x). \end{cases}$$
(17)

Veremos en primer lugar cómo podemos representar la solución u de (17) en el caso libre, $V \equiv 0$. Después daremos una versión del lema de Carleman para el operador hiperbólico 2.3.1 además de incluir su demostración.

El principal teorema del segundo capítulo está enunciado en 2.4.1. Veremos que guarda ligeras diferencias con respecto al teorema 1.4.1 correspondiente al caso elíptico de la ecuación de Schrödinger. Esto se debe a que al aplicar el lema de Carleman 2.3.1 sobre la función g correspondiente aparecen términos que dependen de las dimensiones n_1 y n_2 correspondientes a los vectores x_1 y x_2 . Además aparecerá un factor de la forma $||x_1|^2 - |x_2|^2|$ actuando sobre la solución uque nos sugiera que la norma L^2 de la solución puede estar concentrada alrededor del conjunto $\{(x_1, x_2) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} | |x_1| = |x_2|\}$ cuando $n_1 = n_2$. Esto se puede apreciar en (2.9).

Cerraremos el segundo capítulo tal y como hicimos el primero, mirando el caso particular de la solución periódica de (2.4.1) en dimensión 2. Este último resultado queda recogido en 2.5.1.

Principios de incertidumbre dinámicos

Hemos visto cómo reduciendo las condiciones de dos tiempos a un único tiempo hemos obtenido información acerca de la solución en tiempos posteriores. En la última parte de la tesis seguimos con la misma premisa; es decir, partiendo de condiciones sobre el dato inicial u_0 tratamos de controlar su evolución dinámica. Ahora sin embargo trabajaremos en el contexto de la partícula libre

$$\begin{cases} \partial_t u = \frac{i}{2} \Delta u, \\ u(x,0) = u_0(x), \end{cases}$$
(18)

donde el factor 1/2 ha sido introducido para simplificar los cálculos.

El **capítulo 3** aborda el tema de cómo demostrar (15) partiendo de hipótesis sobre el dato inicial. Para tal fin introducimos los espacios Σ_{δ} que son conjuntos de funciones que satisfacen la siguiente condición

$$\int_{\mathbb{R}^n} |x|^{2\delta} |f(x)|^2 + |D^{\delta}f(x)|^2 dx < +\infty,$$
(19)

donde D^{δ} es una derivada fraccionaria que podemos definir mediante transformadas de Fourier como

$$D^{\delta}f(x) = \int_{\mathbb{R}^n} e^{ix\cdot\xi} |\xi|^{\delta} \hat{f}(\xi) d\xi,$$

para un $\delta > 0$ real sobre el que definiremos ciertas restricciones más adelante.

Veremos que tomando nuestro dato inicial en este espacio su evolución dinámica seguirá estando en el mismo espacio. Recordemos que la transformada de Fourier de la solución u del problema (18) puede escribirse explícitamente como

$$\hat{u}(\xi, t) = u_0(\xi)e^{-\frac{i}{2}t|\xi|^2},$$

de forma que si nuestro dato inicial u_0 está en el espacio Σ_{δ} , claramente se verifica

$$\int_{\mathbb{R}^n} |D^{\delta} u(x,t)|^2 dx = \int_{\mathbb{R}^n} |\xi|^{2\delta} |\hat{u}(\xi,t)|^2 d\xi = \int_{\mathbb{R}^n} |\xi|^{2\delta} |\hat{u}_0(\xi)|^2 d\xi < \infty.$$

Así pues nuestro trabajo será ver que la función h_{δ} que definimos como

$$h_{\delta}(t) = \int_{\mathbb{R}^n} |x|^{2\delta} |u(x,t)|^2 dx, \qquad (20)$$

está acotada para tiempos $t \neq 0$. Este resultado se encuentra en [28], un artículo de J. Nahas y G. Ponce. Nosotros daremos una versión alternativa. Recogemos este resultado en la proposición 3.3.2. La demostración la haremos de manera escalonada. En primer lugar suponiendo que t = 1 y en dimensión 1. La clave de la demostración será escribir la función h_{δ} como

$$\int_{\mathbb{R}} |D^{\delta}(\hat{f}\hat{g})|^2 d\xi$$

donde $\hat{f}(\xi) = e^{-\frac{i}{2}\xi^2}$ y $\hat{g}(\xi) = \hat{u}_0(\xi)$. Usamos el siguiente resultado de C. Kenig, G. Ponce y L. Vega probado en [17]

$$\|D^{\delta}(\hat{f}\hat{g}) - \hat{f}(D^{\delta}\hat{g}) - (D^{\delta}\hat{f})\hat{g}\|_{2} \le c\|\hat{f}\|_{\infty}\|D^{\delta}\hat{g}\|_{2},$$

que junto con el lema de Pitt 3.3.1 e integración por partes nos dará el resultado que buscamos.

Una vez demostrado para tiempo t = 1 usaremos un argumento de dilataciones para generalizarlo a tiempos t > 0. Por último para demostrarlo en dimensiones mayores usaremos el hecho de que la norma euclídea puede controlarse por la norma del máximo y argumentar en una sola variable para la cual ya sabemos que es cierto. Todos los resultados están recogidos en la proposición 3.3.2. Una vez demostrado este teorema, podemos utilizarlo para demostrar (15), ver 3.3.3. Terminamos esta parte generalizando los resultados obtenidos previamente en este capítulo para el siguiente problema no-lineal

$$\begin{cases} i\partial_t u + \Delta u = \mu |u|^{a-1} u, \quad t \in \mathbb{R}, \quad x \in \mathbb{R}^n, \quad \mu = \pm 1, \quad a > 1\\ u(x,0) = u_0(x). \end{cases}$$
(21)

Para ello nos basamos en el artículo [28] de J. Nahas y G. Ponce. En este artículo se busca analizar la evolución dinámica de la solución tal y como hemos hecho nosotros para el caso de la partícula libre con la única diferencia de que los resultados aquí son locales en tiempo a pesar de que bajo ciertas condiciones se pueda dar una versión global de los resultados. Para más detalles sobre este tema el lector puede dirigirse al artículo mencionado. De esta forma damos una versión de la proposición 3.3.2 para el caso no-lineal (21).

Observamos que esta extensión a un caso no-lineal nos permite replantear las hipótesis del teorema 3.1 en [4] siempre y cuando el potencial verifique las condiciones necesarias. Veremos que en nuestro caso necesitamos que nuestra solución u esté en el espacio L^{∞} . Para asegurarnos de ello haremos uso del teorema de inmersión de Sobolev que nos asegura que si la solución pertenece a un espacio de Sobolev $\mathcal{H}^s(\mathbb{R}^n)$ entonces $u \in L^{\infty}$ siempre y cuando s > n/2. Este resultado queda recogido en 3.3.7.

Abordamos de nuevo el tema de cómo demostrar (15) dando exclusivamente condiciones al dato inicial. Sin embargo ahora haremos uso del Teorema Virial. Para ello definimos la siguiente función

$$h(t) = \int_{\mathbb{R}^n} \varphi(x) |u(x,t)|^2 dx,$$

donde consideraremos φ radial y de crecimiento polinomial. Primero analizaremos la función h para un φ general. Una de las propiedades importantes es que podemos calcular la segunda derivada de h en términos de φ de forma que

$$h''(t) = -\frac{1}{4} \int_{\mathbb{R}^n} \Delta^2 \varphi(x) |u(x,t)|^2 dx + \int_{\mathbb{R}^n} \nabla u D^2 \varphi(x) \nabla \bar{u} dx.$$

Esta última expresión nos ayudará a buscar condiciones para poder as egurar la convexidad en h.

Podemos también observar claramente que si tomamos $\varphi(x) = |x|^{2\delta}$ la función *h* se convierte en h_{δ} . Analizaremos este último caso en detalle para $\delta = 1$. Para simplificar la notación utilizaremos *h* en lugar de h_1 cuando hablemos del caso $\delta = 1$.

Este caso guarda ciertas particularidades ya que representa la dispersión de nuestro sistema cuántico y puede representarse de manera explícita mediante las magnitudes que caracterizan la posición y el momento del dato inicial u_0 . Recordemos que $|u(x,t)|^2$ define una función de densidad en el espacio y que gracias a esto y usando la desigualdad de Cauchy-Schwarz obtenemos

$$1 = \int_{\mathbb{R}^n} |u(x,t)|^2 dx \le \frac{2}{n} \left(\int_{\mathbb{R}^n} |xu(x,t)|^2 dx \right)^{1/2} \left(\int_{\mathbb{R}^n} |\nabla u(x,t)|^2 dx \right)^{1/2}, \quad (22)$$

que es nada menos que el Principio de Incertidumbre de Heisenberg que ya hemos mencionado anteriormente. Veremos que esta desigualdad aplicada al instante t = 0 nos permitirá estudiar la dispersión del sistema cuántico en su evolución dinámica. En particular, para nuestro dato inicial definiremos las siguientes cantidades,

$$a^{2} := \int_{\mathbb{R}^{n}} |xu_{0}(x)|^{2} dx, \qquad (23)$$

у

$$b^2 := \int_{\mathbb{R}^n} |\nabla u_0(x)|^2 dx, \qquad (24)$$

de manera que (22) se traduzca en $1 \leq 2ab$ siempre y cuando las cantidades $a \neq b$ sean finitas.

Veremos así que la función h define una parábola convexa que podemos representar como

$$h(t) = a^2 + b^2 t^2,$$

si asumimos que h'(0) = 0.

Usando esta representación de h podemos demostrar (15). Este resultado queda recogido en 3.5.1. Para cerrar este capítulo veremos cómo mediante transformaciones de Galileo podemos generar una nueva familia de soluciones de (18) para ver, mediante un contraejemplo, que las condiciones impuestas sobre el dato inicial u_0 son necesarias.

Para finalizar, en el **capítulo 4** de la tesis daremos un principio de incertidumbre dinámico para la función h_{δ} y buscaremos las soluciones u que minimizan el problema. Hemos visto más arriba que el principio de incertidumbre de Heisenberg puede ser representado mediante la desigualdad $1 \leq 2ab$. Si usamos esto en la definición de nuestra función h vemos que

$$h(t) = a^2 + b^2 t^2 \ge \frac{1}{4b^2} + b^2 t^2,$$

la igualdad únicamente siendo alcanzada cuando 1 = 2ab. Para esta condición sabemos además que el dato inicial debe ser una Gaussiana. Estas funciones aparecen de manera natural cuando hablamos de principios de incertidumbre. De esta

forma cabe esperar que a la hora de plantear principios de incertidumbre dinámicos para la función h_{δ} como hemos mencionado arriba, las Gaussianas aparezcan también como minimizantes del problema. Veremos que efectivamente esto sucede.

Para llevar a cabo este trabajo usaremos un enfoque diferente mediante la representación de nuestra solución como

$$u(x,t) = \rho(x,t)e^{i\theta(x,t)},$$

donde ρ y θ serán funciones reales que dependan de las variables espacio-tiempo y θ además será radial¹. Sustituyendo esta nueva expresión en la ecuación (18) obtenemos el siguiente sistema de ecuaciones diferenciales,

$$\begin{cases} \partial_t \rho + \nabla \theta \cdot \nabla \rho + \frac{1}{2} \rho \Delta \theta = 0, \\ \Delta \rho - \rho (2\partial_t \theta + |\nabla \theta|^2) = 0. \end{cases}$$
(25)

Nuestro trabajo será buscar las soluciones $\rho \ y \ \theta$ que definan u como minimizante del problema. Veremos que la primera ecuación de (25) se puede resolver mediante el método de las características de donde obtendremos ρ en función del dato inicial. Para determinar cuál debe ser este dato inicial usaremos la segunda ecuación, que veremos se puede reducir al problema del oscilador armónico cuyas soluciones son conocidas.

Haremos este análisis para los casos $\delta = 1$ en primer lugar y para $\delta < 1$ después. La ventaja del primer caso es que podemos hacer cálculos explícitos ya que conocemos cómo es la función h. Así, veremos que

$$h^{1/2}(t) \le a + \int_0^t \left(\int_{\mathbb{R}^n} |\rho \nabla \theta|^2 dx \right)^{1/2} ds \tag{26}$$

donde la igualdad se alcanza cuando $\nabla \theta = \lambda(t)x$. Esta última condición junto con la definición de *h* nos permitirá definir la función λ . Como hemos mencionado arriba la segunda ecuación de (25) se puede reducir al problema del oscilador armónico. Analizaremos este problema primero en dimensión 1 y después en dimensiones mayores n > 1 ya que las soluciones varían de un caso a otro.

Para el caso de dimensión 1 veremos que la solución que minimiza el problema se genera tomando como dato inicial las funciones de Hermite. En el caso de dimensiones mayores reescribimos el problema del oscilador armónico utilizando coordenadas polares $x = r\xi$ donde $r = |x| y \xi \in \mathbb{S}^{n-1}$. De esta forma veremos que las soluciones se pueden conseguir mediante separación de variables de forma que

$$u_0(r\xi) = R(r)S(\xi),$$

 $^1 \rm Observamos que ésta no es la representación habitual de Madelung, la cual se difene como<math display="inline">u=\sqrt{\rho}e^{i\theta}$

donde S son armónicos esféricos y R se define mediante polinomios de Laguerre. Todos los resultados de esta sección quedan recogidos en el teorema 4.2.1.

Para el caso $\delta < 1$ estudiamos la desigualdad análoga a (26)

$$h_{\delta}^{1/2}(t) \le a_{\delta} + \delta \int_0^t \left(\int_{\mathbb{R}^n} |x|^{2\delta - 2} \rho^2 |\partial_r \theta|^2 dx \right)^{1/2} ds, \tag{27}$$

donde a_{δ} está definido como

$$a_{\delta}^2 := \int_{\mathbb{R}^n} |x|^{2\delta} |u_0(x)|^2 dx.$$

En este caso tendremos que cerciorarnos de que la cantidad a la derecha de la desigualdad está acotada. Veremos que para esto es suficiente la convexidad de h_{δ} que sólo será posible para dimensiones mayores que 3 y $1/2 < \delta \leq 1$. En cuanto al problema del minimizante veremos que tal y como sucede para el caso $\delta = 1$, se reduce a la resolución del oscilador armónico. Recogemos este resultado en 4.3.1.

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Introduction

A glimpse into Quantum Mechanics

Quantum Mechanics is the part of physics that studies the motion of particles or microobjects. It was born upon the need to give an explanation to some phenomenons to which classical mechanics had no answer at all, such as the radiation of black bodies. In this direction the first steps were made by the German physicist *Max Planck* at the end of the twentieth century.

However, the basis for the theory was not established until the mid 1920's. One of the pioners on the field was the French physicist *Louis de Broglie* who discovered the dual nature of particles, this is, the wave-particle nature. As an example, light was thought to have only wave properties throughout the whole nineteenth century. This idea was later refuted since it was observed that light also had particle-like behaviour.

After *de Broglie*, notorious scientists such as *Erwin Schrödinger*, to whom we owe the name of this thesis or the German mathematician and physicist *Max Born* made their contributions to the theory. The latter was the first to talk about the probabilistic aspect of the theory on an article published in 1926.

We have mentioned two of the most important aspects of Quantum Theory, this is, the wave-particle nature of quantum objects and its probabilistic interpretation. These concepts can be easily understood by the double-slit experiment carried by the English scientist *Thomas Young*. Young wanted to discern the real nature of light. On the second half of the twentieth century the same experiment was carried out by the German physicist *Clauss Jönsson*. This time electrons were used to do the experiment. Later in 1989 a group led by the Japanese physicist *Akira Tonomura* run the same experiment.

The double slit experiment consists of a panel with two slits separated certain distance a and a screen set at distance d from the panel where the electrons hit. Thus equally prepared electrons are shot and the collisions are registered on the screen. When one of the slits is closed the pattern of the collisions shows no intereference at all. In this case a Gaussian-like pattern is observed on the screen

where most colisions occur in front of the open slit. However, when both are open the distribution of the collisions is a little more *messy*.

Suppose now both slits are open. If we shoot one electron at a time we see that it hits the screen at a single point of the screen so its position is clear. Same happens with each one of the electrons that we shoot against the screen. The key point here is that each electron generates a single point but does not scatter as it should be expected by a wave-like object. However the position where an electron hits the screen is completely arbitrary and when we shoot a great amount of them an interference pattern is generated.

The surprising thing is not the variation of points where the electrons hit the screen but the pattern we mentioned. Thanks to this we can clearly identify the areas on the screen where the density of the collisions is higher or on the contrary, the areas where almost no electrons reach as we can observe on the following images:



Figure 2: Image taken from [14], p. 13, corresponding to the double slit experiment run by Akira Tonomura's team in 1989.

The first picture corresponds to the distribution of 150 electrons and we cannot distinguish any clear pattern. On the other hand, the last image corresponds to the distribution of 160.000 electrons and in this case we can clearly identify the areas with more density.

When we talk about the wave-nature of electrons we are referring to this intereference pattern. Of course if we shoot a single electron we cannot predict where on the screen will hit but we can assign a probability to each of the points. To do so we use a function that will characterize the pattern we mentioned earlier. This function is precisely the *wave function* that represents our system of electrons.

This function is evaluated on $x \in \mathbb{R}^n$, that should be understood as the possible points where the particle can be found, and its time evolution will be determined by *Schrödinger's equation*. It should be mentioned that this function does not represent a single particle but the statistical behaviour of the whole system of particles which we refer to as **quantum system**.

Although this might seem like an over-simplification we can see the dual nature of particles the following way: a single particle behaves as such but a succession of them will show a wave-like behaviour.

On this thesis we refer to the wave function that characterizes the quantum system as u = u(x, t) where $x \in \mathbb{R}^n$ as we have already mentiond and t will be the time parameter that will determine the dynamical evolution of the system. The function u has thus all the information about the system. In particular, $|u(x, t)|^2$ describes a probability density function related to the position. It thus makes sense to assume that

$$\int_{\mathbb{R}^n} |u(x,t)|^2 dx = 1,$$

for every t. This means that the probability to find a particle somewhere in space is absolute.

It is clear that when we talk about quantum systems we cannot measure with total certainty like we do on classical mechanics. On the latter the behaviour of particles is uniquely determined by its position and momentum values at a given time t. The most we can do now is to calculate probabilities of these magnitudes. Up to this point we have talked about the position of a particle but there are more physical magnitudes we could mention.

In Quantum Mechanics the physical quantities (position, momentum, energy,...) are represented by self-adjoint operators defined on a Hilbert space \mathcal{H} . Recall first that the inner product between two vectors on a Hilbert space \mathcal{H} is defined by

$$\langle u, v \rangle = \int_{\mathbb{R}^n} u \bar{v} dx, \quad \forall u, v \in \mathcal{H}(\mathbb{R}^n).$$

Definition. Let S be a linear operator defined on a Hilbert space \mathcal{H} . The adjoint operator of S, named S^* is the operator that satisfies

$$\langle u, Sv \rangle = \langle S^*u, v \rangle,$$

for every $v \in \mathcal{D}(S)$ and $u \in \mathcal{D}(S^*)$.

Definition. A linear operator S is said to be hermitian if

$$Su = S^*u, \quad \forall u \in \mathcal{D}(S).$$

If further $\mathcal{D}(S) = \mathcal{D}(S^*)$ we can strictly say that $S = S^*$. In this case we say S is **self-adjoint**.

Definition. Likewise, we say the linear operator A is anti-hermitian if

$$Au = -A^*u, \quad \forall u \in \mathcal{D}(A).$$

Suppose there is a particle moving along the real line \mathbb{R} . We know from the probability theory that the *expected value* of the position is given by

$$\int_{\mathbb{R}} x |u(x,t)|^2 dx,$$

for any fixed time t. If we define S = x as the position operator we see that we can write the expectation of the position as the inner product of the corresponding Hilbert space, say

 $\langle Su, u \rangle$.

One of the main ideas of quantum theory is to represent the expected value of different physical magnitudes using operators and the inner product as we have done for the case of the position.

Another important magnitude that we will talk about in this thesis is the momentum. Momentum is represented by the operator $S = -i\partial_x$ in dimension 1 or $S = -i\nabla$ in higher dimensions. One of the characteristics of the momentum of a quantum system is that its information is codified on the frequency space so that the momentum of a single particle is given by $p = \hbar \xi$ where \hbar is *Planck's constant* and ξ is the frequency variable. This observation is important since it tells us that there is a special relation between the wave function u and its Fourier transform. Moreover, we will see that this relation implies the imposibility to measure position and momentum simultaneously with high accuracy. This phenomenon is known as the *Uncertainty Principle* and it is another fundamental topic of this thesis.

We define the Fourier Transform of a function f as

$$\hat{f}(\xi) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-ix \cdot \xi} f(x) dx,$$

where $x \cdot \xi = x_1 \xi_1 + \ldots + x_n \xi_n$ is the scalar product.

Thus it makes sense to construct u as the superposition of functions defined on the frequency space via the inverse Fourier transform

$$u(x,t) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{ix\cdot\xi} \hat{u}(\xi,t) d\xi.$$
Schrödinger's equation

It is clear that there are several differences between classical and quantum mechanics. We mentioned that in the former a physical system is totally determined by its position and momentum at certain time t_0 . We can even talk about the dynamical evolution of the system by describing trajectories, which is certainly not possible in a quantum scheme.

However it still makes sense to think that the quantum system evolves in time and so will the wave function u. This being so we say that the state of the system is described by $u_t(x) = u(x, t)$ where t plays the role of the time parameter. How can we characterize the evolution in time of the system if we cannot talk about trajectories like we do on the classical context?

The job is done by the equation presented by the Austrian physicist *Erwin* Schrödinger in 1926

$$i\hbar\frac{\partial}{\partial t}u(x,t) = Hu(x,t),$$

known as the time dependent Schrödinger equation where \hbar is *Planck's constant* and *H* is the *Hamiltonian* that characterizes the energy of the system.

The version of the equation given above is the version in physics we can find in the literature. In this thesis we work in a mathematical context of the problem so we instead write it as an initial value problem

$$\begin{cases} \partial_t u(x,t) = i(\Delta u(x,t) + V(x,t)u(x,t)), & x \in \mathbb{R}^n, t \in \mathbb{R} \\ u(x,0) = u_0(x), \end{cases}$$
(28)

where V is the potential and Δ is the Laplacian defined as

$$\Delta = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}.$$

We refer to the particular case where no potential is involved as the free-particle case. Moreover, when we work in this context we introduce a factor 1/2 so that calculations are more simple. The equation is thus

$$\partial_t u = \frac{i}{2} \Delta u. \tag{29}$$

For the case of the free particle we can compute the solution of Schrödinger's problem explicitly using properties of the Fourier transform. Thus equation (29) becomes

$$\partial_t \hat{u}(\xi,t) = -\frac{i}{2} |\xi|^2 \hat{u}(\xi,t),$$

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which we solve and get

$$\hat{u}(\xi, t) = \hat{u}_0(x)e^{-\frac{i}{2}t|\xi|^2}.$$

Using now the inversion formula of the Fourier transform we can write the solution u of (29) as

$$u(x,t) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-ix\cdot\xi} \hat{u}(\xi,t) d\xi = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-ix\cdot\xi} e^{-\frac{i}{2}t|\xi|^2} \hat{u}_0(\xi) d\xi.$$

Or in a more refined way as

$$u(x,t) = e^{it\Delta}u_0(x) = \frac{1}{(2\pi i t)^{n/2}} \int_{\mathbb{R}^n} e^{i\frac{|x-\xi|^2}{2t}} u_0(\xi) d\xi,$$
(30)

where $i^{1/2} = e^{i\pi/4}$ when t > 0. If we consider t < 0 then we should take its conjugate $i^{1/2} = e^{-i\pi/4}$.

This representation of the solution also tells us that Schrödinger's equation is a dispersive equation.

Another feature of the solution of the free Schrödinger equation is that if u is a solution to (29) then so are its spatial derivatives whenever they exist.

Uncertainty Principles

We have talked about how in the context of quantum mechanics it is impossible to measure with high accuracy the position and the momentum of the system. This phenomenon is known as the Uncertainty Principle and it was stated in [47] by the German physicist *Werner Karl Heisenberg* in 1927.

In mathematics Heisenberg's Uncertainty Principle can be expressed as the following inequality

$$\frac{2}{n} \left(\int_{\mathbb{R}^n} |xf(x)|^2 dx \right)^{1/2} \left(\int_{\mathbb{R}^n} |\nabla f(x)|^2 dx \right)^{1/2} \ge \int_{\mathbb{R}^n} |f(x)|^2 dx.$$
(31)

We can obtain (31) as a particular case of a more abstract Uncertainty Principle as we shall see next.

Let \mathcal{H} be a Hilbert space and let S and A be a hermitian and anti-hermitian operators respectively, i.e. for a suitable function ψ

$$\langle S\psi,\psi\rangle = \langle\psi,S\psi\rangle, \quad \langle A\psi,\psi\rangle = -\langle\psi,A\psi\rangle.$$

Then for the operator S + A and $\psi \in \mathcal{D}(S) \cap \mathcal{D}(A)$ we get

$$0 \leq ||(A+S)\psi||^{2} = \langle S\psi, S\psi \rangle + \langle A\psi, A\psi \rangle + \langle S\psi, A\psi \rangle + \langle A\psi, S\psi \rangle$$
$$= \langle S\psi, S\psi \rangle + \langle A\psi, A\psi \rangle + 2Re\langle S\psi, A\psi \rangle$$
$$= \langle S\psi, S\psi \rangle + \langle A\psi, A\psi \rangle + \langle (SA - AS)\psi, \psi \rangle.$$

Therefore,

$$-\langle (SA - AS)\psi, \psi \rangle \le ||S\psi||^2 + ||A\psi||^2.$$
(32)

If we do the same calculation but instead of A we use -A we get

$$\langle (SA - AS)\psi, \psi \rangle \le ||S\psi||^2 + ||A\psi||^2, \tag{33}$$

and combining (32) and (33) we see that

$$|\langle (SA - AS)\psi, \psi \rangle| \le ||S\psi||^2 + ||A\psi||^2.$$
 (34)

Let $\lambda > 0$ and define

$$\tilde{A} = \lambda A, \qquad \tilde{S} = \frac{1}{\lambda}S.$$

If we now plug \tilde{A} and \tilde{S} in (33) we get

$$|\langle (SA - AS)\psi, \psi\rangle| \le \frac{1}{\lambda^2} ||S\psi||^2 + \lambda^2 ||A\psi||^2.$$
(35)

Since λ was arbitrary we take $\lambda^2 = \frac{||S\psi||}{||A\psi||}$ so that equation (35) becomes

$$|\langle (SA - AS)\psi, \psi \rangle| \le 2||S\psi|| \ ||A\psi||. \tag{36}$$

Inequality (36) is precisely the Uncertainty Principle. On the other hand, this inequality becomes an identity when

$$(S+A)\psi = 0.$$

As an application of the Uncertainty Principle we can choose $\mathcal{H} = L^2(\mathbb{R})$ and consider the operators

$$S\psi = x\psi, \qquad A\psi = \frac{d}{dx}\psi = \psi'.$$

For this case we obtain Heisenberg's Uncertainty Principle we mentioned earlier. If we now calculate the commutator of these operators we get

$$(SA - AS)\psi = \left(x\frac{d}{dx} - \frac{d}{dx}x\right)\psi = x\psi' - (x\psi)'$$
$$= x\psi' - \psi - x\psi' = -\psi.$$

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Observe that by (36),

$$-\langle (SA - AS)\psi, \psi \rangle = \langle \psi, \psi \rangle \le 2\left(\int |x\psi|^2\right)^{1/2} \left(\int |\psi'|^2\right)^{1/2}.$$
 (37)

And we have an identity only if $\psi' = -x\psi$, this is, only if the sum of the operators is identically zero as we mentioned before. If we solve the ordinary differential equation we get $\psi_0 = Ce^{-x^2/2}$ which is precisely the function for which (37) is an identity. We can thus say that ψ_0 is a minimizer of the problem. We see that Gaussian functions appear naturally when we try to find minimizers of Uncertaity Principles. On the other hand we see that

$$0 = \langle (A+S)\psi, (A+S)\psi \rangle = \langle (S-A)(S+A)\psi, \psi \rangle = \langle \left(S^2 - A^2 + SA - AS\right)\psi, \psi \rangle,$$

so the function ψ_0 satisfies the following differential equation

$$-\frac{d^2}{dx^2}\psi_0(x) + x^2\psi_0(x) = \psi_0(x).$$

We thus see that ψ_0 is an eigenfunction of the harmonic oscilator problem with associated eigenvalue $\lambda = 1$.

The Uncertainty Principle can also be interpreted in terms of a function and its Fourier transform. Recall one of the fundamental results in Fourier theory, the so called *Plancherel's identity*. This identity tells us that the L^2 norm of a function and its Fourier transform are the same

$$\int_{\mathbb{R}^n} |f(x)|^2 dx = \int_{\mathbb{R}^n} |\hat{f}(\xi)|^2 d\xi.$$

Using this together with other properties of the Fourier transform we can write (31) as

$$\frac{2}{n} \left(\int_{\mathbb{R}^n} |xf(x)|^2 dx \right)^{1/2} \left(\int_{\mathbb{R}^n} |\xi \hat{f}(\xi)|^2 d\xi \right)^{1/2} \ge \int_{\mathbb{R}^n} |f(x)|^2 dx.$$

The identity attained when both integrals on the left hand side of the inequality are proportional to one another. Thus the functions that minimize the problem are functions whose Fourier transform is the original function which is precisely a property of Gaussian functions.

It is clear that Gaussians play a fundamental role in the framework of Uncertainty Principles and the decay of a function and its Fourier transform. Following up we introduce Hardy's Uncertainty Principle [11], named after the British mathematician Godfrey H. Hardy. The result says

$$|f(x)| \le Ce^{-\alpha|x|^2}, \quad |\hat{f}(\xi)| \le Ce^{-\beta|x|^2}, \quad \alpha\beta > \frac{1}{4} \Rightarrow f \equiv 0.$$
(38)

Further if $\alpha\beta = 1/4$ then f has to be a Gaussian $f(x) = Ce^{-\alpha|x|^2}$. The proof of this result uses techniques of complex analysis and we will not go deeper on the details. However the reader can refer to [34], [35] y [36] to learn more about it. Hardy's Uncertainty Principle has been largely studied for a long time, extended to higher dimensions and has also been posed in more general contexts by authors like Bonami-Demange-Jaming, Cowling-Price, Hörmander and Sitaram-Sundari-Thangavelu in [37], [38], [39], [40], [41], [42], [43] among others.

We can relate Hardy's Uncertainty Principle to the solution of Schrödinger's problem. If we write (30) as

$$u(x,t) = \frac{1}{(2\pi i t)^{n/2}} e^{i\frac{|x|^2}{2t}} \left(\widehat{e^{i\frac{|\cdot|^2}{2t}} u_0} \right) \left(\frac{x}{t}\right), \tag{39}$$

we observe that the solution of the problem is written in terms of the Fourier transform of the initial data properly modulated. This implies that giving size conditions on the solution u in two times is equivalent to giving size conditions to u and the transform of the initial data. Under this premise we can give a version of Hardy's Uncertainty Principle that grants a qualitative result about the solution u,

If
$$e^{\frac{|x|^2}{\beta^2}}u_0(x), e^{\frac{|x|^2}{\alpha^2}}e^{it\Delta}u_0(x) \in L^2(\mathbb{R}^n) \text{ y } \alpha\beta \leq 4t$$
, then $u_0 \equiv 0.$ (40)

In a series of articles by L. Escauriaza, C.E. Kenig, G. Ponce and L. Vega they give unique continuation results that grant qualitative properties of the solution as the one mentioned above. Some of the articles are [4], [6], [10] and the main motivation is Hardy's Uncertainty Principle. The goal of these articles is to give similar results but using real variable arguments and considering perturbative scenarios, this is, cases where the potential is non-zero. For this purpose they give conditions on the solution at two times and a size condition on the potential, say

$$\lim_{R \to +\infty} \int_0^1 \|V(t)\|_{L^{\infty}\left(\mathbb{R}^d \setminus B_R\right)} dt = 0,$$

where B_R is the ball of radius R, so that the only solution to the problem is the trivial $u \equiv 0$. Moreover they use these results on non-linear problems such as

$$i\partial_t u + \Delta u = \pm |u|^2 u,$$

to give uniqueness results.

One of the techniques used in these series of papers is the use of Carleman's estimates which allow to work in perturbative contexts. In particular in [4] the following Carleman inequality is used

$$\frac{\sigma^{3/2}}{c_n R^2} \left\| e^{\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} g \right\|_2 \le \left\| e^{\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} \left(i\partial_t + \Delta \right) g \right\|_2, \tag{41}$$

to prove that the only solution that decays faster than $e^{-a|x|^2}$ for a sufficiently large is the trivial solution. In (41) c_n is a constant that only depends on the dimension, the function $\varphi : [0,1] \longrightarrow \mathbb{R}$ is a smooth function, $\sigma \ge c_n R^2$ and g is a function that belongs in the space $C_0^{\infty}(\mathbb{R}^{n+1})$ whose support is contained in the set

$$\left\{(x,t): \left|\frac{x}{R} + \varphi e_1\right| \ge 1\right\}.$$

Up to this point we have talked about Uncertainty Principles related to the (Gaussian) decay of a function and its Fourier transform. Another version of them says that a function and its transform cannot be simultaneously concentrated somewhere in space. This means that if a non-zero function f has compact support then its Fourier Transform cannot satisfy a condition like $\hat{f}(\xi) = \mathcal{O}(e^{-\epsilon|\xi|})$ for any $\epsilon > 0$.

This is due to the fact that $\hat{f}(\xi) = \mathcal{O}(e^{-\epsilon|\xi|})$ implies that f has an analytic extension on the band $\{z \in \mathbb{C}^n : |Im(z)| < \epsilon\}$. These kind of Uncertainty Principles are named after the British mathematician *Raymond Paley* and the American philosopher and mathematician *Norbert Wiener*. We refer to them as Uncertainty Principles of Paley-Wiener type. These principles allow to characterize functions with compact support in terms of the analytic properties of their Fourier Transform.

In other article by C.E. Kenig, G. Ponce and L. Vega [7] they once again look for conditions at two times to conclude that the solution u must be identically zero. The conditions this time are Paley-Wiener type conditions. The strategy followed in this article combines the use of Carleman's estimate with Appell's Conformal transformations. These transformations generate a new family of solutions of (28) by making dilations in both time and space variables. Defining the function g of Carleman's lemma in a proper way, Appell's transformations allow us to adjust the integration regions in terms of the dilation parameters.

This idea is used in **chapter 1** of the thesis to give quantitative results of the solution u of (28). Besides, we are going to reduce the conditions from two times to just one. This being so we focus on the initial data u_0 and find suitable conditions on this function so that we can get information about its dynamic evolution. The starting point is a result from article [4]. More precisely Theorem 3.1 in this paper. The goal is to find lower bounds to the solution u of

$$i\partial_t u + \Delta u + V u = 0, \quad t \in [0,1], \quad x \in \mathbb{R}^n,$$

and its gradient on a region of the form $\{R - 1 \leq |x| \leq R\} \times [0, 1]$ where R depends on the norm of u and the size of the potential V. One of the hypothesis

of the theorem says that on a space-time cylinder around the origin and near times $t \sim 1/2$ the L^2 norm of the solution is controlled from below, this is,

$$\int_{1/2-1/8}^{1/2+1/8} \int_{|x|<1} |u|^2(x,t) dx dt \ge 1.$$
(42)

The outcome of the theorem is the following

$$\delta(R) \equiv \left(\int_0^1 \int_{R-1 < |x| < R} \left(|u|^2 + |\nabla_x u|^2 \right)(x, t) dx dt \right)^{1/2} \ge c e^{-cR^2}, \qquad (43)$$

where c = c(n), this is, the decay of the solution cannot be greater than the Gaussian. The main result of chapter one is stated in 1.4.1. The proof of the main theorem follows the same scheme as the one of theorem 3.1 in [4]. The difference is that we introduce Appell's Conformal transformations as we mentioned. Thanks to this trick we give lower bounds of the H^1 norm of the solution locally for small times on a spatial region that depends on time as well.

We will see that the new region of integration is dynamic in the sense that it varies with respect to certain parameters. These parameters are later used to give uniqueness results of the problem. These results are stated in theorems 1.4.2 and 1.4.3.

Another advantage of theorem 1.4.1 is that allows complex potentials depending on the space and time variables. This fact gives rise to non-linear problems that we can study as long as a nice well-posedness theory is available. This being so we can treat problems of the form

$$\partial_t u = i \left(\Delta u + f \left(|u|^2 \right) u \right),$$

for f real and f(0) = f'(0) = 0.

We will also see that by using Carleman's inequality the gradient term appears on the outcome so that we can talk about the H^1 norm of the solution. It is however natural to wonder whether the gradient term is needed. If this were the case we could have observability results as the ones shown in [45], [46]. The problem is that the Schrödinger problem we work with allows potentials depending on both space and time variables. In [1] they give n observability result in $\mathbb{T}^n := (\mathbb{R}/2\pi\mathbb{Z})^n$ for potentials that does not depend on time. Following the same ideas in [45] they give an observability result for the problem

$$i\partial_t u(t,z) = (-\Delta + V(z))u(t,z), \quad z \in \mathbb{T}^2,$$

where $\mathbb{T}^2 := \mathbb{R}^2 / A\mathbb{Z} \times B\mathbb{Z}$, $A, B \in \mathbb{R} \setminus \{0\}$ and the potential $V \in \mathcal{C}(\mathbb{T}^2)$ is real.

We close the first chapter of the thesis analyzing the case of a periodic solution. We will see how 1.4.1 changes for this type of solutions and how it affects the region where we observe both the solution and its gradient.

In chapter 2 of the thesis, following a suggestion by professor J. Marzuola, we extend the results obtained on the first chapter for the hyperbolic Schrödinger operator, so that the problem in hand is

$$\begin{cases} \partial_t u = (\Delta_1 - \Delta_2 + V(x, t))u\\ u(x, 0) = u_0(x). \end{cases}$$
(44)

First we see how we can represent the solution u of (44) when $V \equiv 0$. After this we give a version of Carleman's lemma for the hyperbolic case 2.3.1 and we include the proof of it.

The main theorem of chapter 2 is stated in 2.4.1. We see that the outcome of the theorem is slightly different from the one shown on the elliptic version. This is due to the fact that when we apply Carleman's lemma 2.3.1 on the function gwe have terms depending on dimensions n_1 and n_2 of the corresponding vectors x_1 and x_2 . Moreover, we will see that a factor $||x_1|^2 - |x_2|^2|$ appears acting on the solution u which suggests that the L^2 norm of the solution might be concentrated around the set $\{(x_1, x_2) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \mid |x_1| = |x_2|\}$ when $n_1 = n_2$. This can be seen in (2.9).

We finish the second chapter analyzing the case of the periodic solution like we did on the previous one. In this case we give the result in dimension 2. This last theorem is stated in 2.5.1.

Dynamical Uncertainty Principles

We have seen that conditions at time t = 0 have granted us information about the solution at times t > 0. In the last part of the thesis we continue with the same idea, this is, starting with conditions on the initial data u_0 we try to control its dynamical evolution. However now we work on the free-particle case, say

$$\begin{cases} \partial_t u = \frac{i}{2} \Delta u, \\ u(x,0) = u_0(x), \end{cases}$$
(45)

where the factor 1/2 has been introduced by convenience.

In chapter 3 we find conditions on the initial data u_0 to prove (42). To carry on this task we introduce the Σ_{δ} space. This space contains functions satisfying the following condition

$$\int_{\mathbb{R}^n} |x|^{2\delta} |f(x)|^2 + |D^{\delta} f(x)|^2 dx < +\infty,$$
(46)

where D^{δ} is a fractional derivative that we define via Fourier transformations as

$$D^{\delta}f(x) = \int_{\mathbb{R}^n} e^{ix\cdot\xi} |\xi|^{\delta} \hat{f}(\xi) d\xi,$$

for $\delta > 0$ real. We will see how restrictive the conditions on the parameter δ are depending on the context we work in.

First we see that if we consider the initial data u_0 belong in the space Σ_{δ} , then its evolution in time will also belong in it. Recall that the Fourier transform of the solution of (45) can be explicitly written as

$$\hat{u}(\xi, t) = u_0(\xi) e^{-\frac{i}{2}t|\xi|^2}.$$

This means that if $u_0 \in \Sigma_{\delta}$ then

$$\int_{\mathbb{R}^n} |D^{\delta} u(x,t)|^2 dx = \int_{\mathbb{R}^n} |\xi|^{2\delta} |\hat{u}(\xi,t)|^2 d\xi = \int_{\mathbb{R}^n} |\xi|^{2\delta} |\hat{u}_0(\xi)|^2 d\xi < \infty.$$

Thus our job will be to verify that the function h_{δ} defined as

$$h_{\delta}(t) = \int_{\mathbb{R}^n} |x|^{2\delta} |u(x,t)|^2 dx, \qquad (47)$$

is bounded for times $t \neq 0$. This result can be found in [28], an article by J. Nahas and G. Ponce. We give an alternative proof. The proposition is written in 3.3.2. The proof of this proposition is given one step at a time. First we suppose that t = 1 and that the dimension is also 1. The key point of the proof is to write the function h_{δ} as

$$\int_{\mathbb{R}} |D^{\delta}(\hat{f}\hat{g})|^2 d\xi,$$

where $\hat{f}(\xi) = e^{-\frac{i}{2}\xi^2}$ and $\hat{g}(\xi) = \hat{u}_0(\xi)$. We also use the following result by C. Kenig, G. Ponce and L. Vega found in [17]

$$\|D^{\delta}(\hat{f}\hat{g}) - \hat{f}(D^{\delta}\hat{g}) - (D^{\delta}\hat{f})\hat{g}\|_{2} \le c\|\hat{f}\|_{\infty}\|D^{\delta}\hat{g}\|_{2},$$

that together with Pitt's lemma 3.3.1 and integration by parts grants the desired result.

Once it is proved for t = 1 we use a dilation argument to generalize it to times t > 0. Finally, to generalize the result to higher dimensions we recall that the euclidean norm is controlled by the norm of the maximum. This being so we can use the fact that the result is true in dimension one to conclude what we want. All the computations lead to proposition 3.3.2 that we use to prove (42), cf 3.3.3.

We finish this part generalyzing the results obtained previously in this chapter for the following non-linear problem

$$\begin{cases} i\partial_t u + \Delta u = \mu |u|^{a-1} u, \quad t \in \mathbb{R}, \quad x \in \mathbb{R}^n, \quad \mu = \pm 1, \quad a > 1\\ u(x,0) = u_0(x). \end{cases}$$
(48)

For this purpose we refer to [28], an article by J. Nahas and G. Ponce. In this paper they analyze the dynamical evolution of the solution like we have done for the free particle case. The difference is that the results of the mentioned paper are local in time even though under certain conditions we can also give a global version of them. This being so we give a version of proposition 3.3.2 for the non-linear problem (48).

Observe that this extension to the non linear equation allows us to rephrase the hypothesis in theorem 3.1 in [4] as long as the conditions on the potential are satisfied. We thus need that the solution u belongs in L^{∞} . This can be done by using Sobolev's embedding theorem. Indeed, if the solution u belongs in a Sobolev space $H^s(\mathbb{R}^n)$ then $u \in L^{\infty}$ if s > n/2. This result is stated in 3.3.7.

We go back to finding conditions on the initial data to prove (42). However now we use the Virial Theorem to give a different approach to the matter. For this purpose we define the following function

$$h(t) = \int_{\mathbb{R}^n} \varphi(x) |u(x,t)|^2 dx,$$

where we consider φ radial with polynomial growth. First we analyze the function h for a general function φ . One of the important features of h is that we can calculate its second derivative in terms of φ as

$$h''(t) = -\frac{1}{4} \int_{\mathbb{R}^n} \Delta^2 \varphi(x) |u(x,t)|^2 dx + \int_{\mathbb{R}^n} \nabla u D^2 \varphi(x) \nabla \bar{u} dx.$$

This expression will help us find convexity conditions for h.

It is also clear that if we choose $\varphi(x) = |x|^{2\delta}$ then $h = h_{\delta}$. We thus focus on the particular case $\delta = 1$. To ease the notation we use h when we refer to the case $\delta = 1$.

This case has some particularities which we will extensely point out. From a physical point of view the function h describes the dispersion of the quantum system and it can be explicitly described in terms of the position and momentum of the initial data u_0 . Recall that $|u(x,t)|^2$ defines a density function in space. Thus using Cauchy-Schwarz's inequality we obtain

$$1 = \int_{\mathbb{R}^n} |u(x,t)|^2 dx \le \frac{2}{n} \left(\int_{\mathbb{R}^n} |xu(x,t)|^2 dx \right)^{1/2} \left(\int_{\mathbb{R}^n} |\nabla u(x,t)|^2 dx \right)^{1/2}, \quad (49)$$

which is nothing but Heisenberg's Uncertainty Principle mentioned earlier. We will see that this inequality at time t = 0 will let us study the dispersion of the system in its dynamical evolution. For convenience we thus introduce the following quantities

$$a^{2} := \int_{\mathbb{R}^{n}} |xu_{0}(x)|^{2} dx,$$
(50)

and

$$b^2 := \int_{\mathbb{R}^n} |\nabla u_0(x)|^2 dx, \tag{51}$$

so that (49) is written as $1 \leq 2ab$ as long as a and b are finite.

We will thus see that the function h defines a convex parabola that can be represented as

$$h(t) = a^2 + b^2 t^2,$$

if we consider h'(0) = 0.

Using this definition of the function h we prove (42). The result is stated in 3.5.1. To finish up the chapter we see that using Galilean transformations we can generate a family of solutions of (45) to see, by a counterexample, that conditions set upon the initial data u_0 are necessary.

And lastly in **chapter 4** of the thesis we present a dynamical Uncertainty Principle for the function h_{δ} and we find solutions u that minimize this problem. We have seen above that Heisenberg's Uncertainty Principle may be represented by the inequality $1 \leq 2ab$. If we use this on the definition of our function h we see that

$$h(t) = a^2 + b^2 t^2 \ge \frac{1}{4b^2} + b^2 t^2,$$

where equality is only attained when 1 = 2ab. For this to happen we further know that the initial data has to be the Gaussian function. We have also mentioned that Gaussians appear naturally when we deal with Uncertainty Principles. It is not naive to expect that for Uncertainty Principles related to our function h_{δ} the Gaussian function will also appear as a minimizer. We will see that this is indeed true.

To carry out this task we take a different approach and represent the solution u of Schrödinger's problem as

$$u(x,t) = \rho(x,t)e^{i\theta(x,t)},$$

where ρ and θ are real functions that depend on space-time variables and θ will be radial². If we plug in the exponential definition of u in (45) we get the following

²Observe that this is not the same as the Madelung representation which is given by $u=\sqrt{\rho}e^{i\theta}$

system of partial differential equations

$$\begin{cases} \partial_t \rho + \nabla \theta \cdot \nabla \rho + \frac{1}{2} \rho \Delta \theta = 0, \\ \Delta \rho - \rho (2 \partial_t \theta + |\nabla \theta|^2) = 0. \end{cases}$$
(52)

Our job will be to find the functions ρ and θ defining u as a minimizer of the problem. We see that the first equation of (52) can be solved by the method of characteristics from where we obtain ρ in terms of the initial data u_0 . Next we solve the second equation in (52) to determine what u_0 has to be. We will see that the problem is reduced to solving the harmonic oscilator problem for which the solutions are known.

We do the analysis for the case $\delta = 1$ first and $\delta < 1$ after. The former has the advantage that the calculations are explicit since we know the function h. Thus we see that

$$h^{1/2}(t) \le a + \int_0^t \left(\int_{\mathbb{R}^n} |\rho \nabla \theta|^2 dx \right)^{1/2} ds \tag{53}$$

where equality holds if $\nabla \theta = \lambda(t)x$. This condition together with the definition of h will let us define the function λ . As we have mentioned, the second equation in (52) can be reduced to the harmonic oscilator problem. We analyze this problem first in dimension 1 and in higher dimensions later since not both are solved equally.

For the 1 dimensional case we will see that the functions minimizing the problem in hand are the ones generated by the Hermite functions. For the n dimensional case the solution to the harmonic oscilator problem can be rewritten using polar coordinates so that $x = r\xi$ where r = |x| and $\xi \in \mathbb{S}^{n-1}$. Making this change of variables we see that the harmonic oscilator problem can be solved by separation of variables so that

$$u_0(r\xi) = R(r)S(\xi),$$

where S are spherical harmonics and R is defined by Laguerre polynomials. All the results of this section are stated in theorem 4.2.1.

For the case $\delta < 1$ we study the analogous to (53)

$$h_{\delta}^{1/2}(t) \le a_{\delta} + \delta \int_0^t \left(\int_{\mathbb{R}^n} |x|^{2\delta - 2} \rho^2 |\partial_r \theta|^2 dx \right)^{1/2} ds, \tag{54}$$

where a_{δ} is defined as

$$a_{\delta}^2 := \int_{\mathbb{R}^n} |x|^{2\delta} |u_0(x)|^2 dx.$$

For this case we have to make sure that the integral on the right hand side is bounded. We see that in order to prove this it suffices to find conditions so that h_{δ} is convex. We see that this is true when we work in dimension $n \geq 3$ and parameter δ satisfies $1/2 < \delta \leq 1$. As for the minimizing problem we see that the problem reduces to solving the harmonic oscilator problem like we did for the case $\delta = 1$. The last theorem of the thesis takes this last result in 4.3.1.

Chapter 1

Lower bounds for the solution of the Schrödinger equation

1.1 Introduction

As mentioned before, microscopic objects have a dual nature, i.e. a wave-particle nature. This property makes the motion of these objects somewhat unpredictable and therefore it is difficult to measure with accuracy the behaviour of quantum systems. This being so, the best we can do is to try to estimate the probability to find a particle somewhere in space at a given time or time interval. We work in the context of Schrödinger's initial value problem with a potential, say

$$\begin{cases} \partial_t u = i(\Delta u + V(x,t)u) \\ u(x,0) = u_0(x) \end{cases}$$
(1.1)

where V(x,t) will be considered bounded and not necessarily real. The function u_0 is what we call the initial data, this is, the state of the system at time t = 0. This function gives an idea of how the particle evolves at future times so it is interesting to study its nature and decide what conditions should it satisfy to have some control over the solution u of the equation. This will be the main topic not only on the first chapter but also throughout the whole thesis.

The main goal of this chapter is to find conditions to estimate the probability to find the particle described by u somewhere in space, or rather, to ensure that this probability is not 0. This is directly connected to unique continuation results which serve as a motivation. When analyzing the behaviour of the solution of Schrödinger's equation, we encounter two possible scenarios. It may happen that the only solution to the problem is the trivial one. This kind of results are related to qualitative unique continuation properties. There is a number of articles by L. Escauriaza, C. Kenig, G. Ponce and L. Vega that talk about this problem. Some of them are [4], [5], [6], [10], [11]. We are going to mention some of the results found on these papers.

One of the most important properties in Quantum Mechanics is the Uncertainty Principle. This principle plays a fundamental role when studying the behaviour of quantum systems because it establishes a strong connection between a function and its Fourier Transform. It is also directly connected to the problems we mentioned earlier, say, the quantification of the solution. In mathematics, the Uncertainty Principle may be expressed as follows:

$$\frac{2}{n} \left(\int_{\mathbb{R}^n} |xf(x)|^2 dx \right)^{1/2} \left(\int_{\mathbb{R}^n} |\nabla f(x)|^2 dx \right)^{1/2} \ge \int_{\mathbb{R}^n} |f(x)|^2 dx, \tag{1.2}$$

where n is the space dimension and f is a suitable function. This inequality has also an interpretation from the mathematical point of view. This is that a function and its Fourier Transform cannot both decay too fast simultaneously. We define the Fourier Transform of a function f as

$$\hat{f}(\xi) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-i\xi \cdot x} f(x) \, dx,$$

where $\xi \in \mathbb{R}^n$.

The main result of this chapter 1.4.1 is motivated by results concerning lower bounds to the solution u of (1.1). The idea is to find conditions on the initial data u_0 so that the particle described by u is observable on some space-time region of space, observable meaning that its L^2 norm is quantified.

This chapter is organized as follows. First we talk about Uncertainty Principles and the connection with Schrödinger's problem via the Fourier Transform. Then we talk about the motivation to study the quantification of the solution u and the needed tools to build the theory, together with the proofs. The last part of this chapter addresses the similarities with observability inequalities and the geometry of the observability region described on the main result. We complete this last section by analyzing the particular case of the periodic solution of (1.1).

1.2 Uncertainty Principles

An uncertainty principle is a mathematical result that gives limitations on the simultaneous localization of a function and its Fourier transform. There are many statements of that nature, the most famous being due to Heisenberg-Pauli-Weil when localization is measured in terms of smallness of dispersions and to Hardy when localization is measured in terms of Gaussians.

Uncertainty Principles

As mentioned before, there is a general way to see the Uncertainty Principle by using operators. The particular case where the symmetric operator is S = xand the anti-symmetric operator is $\mathcal{A} = \nabla$, position and momentum operators respectively, is connected to (1.2). Another way to read the Uncertainty Principle is the following:

$$\frac{2}{n} \left(\int_{\mathbb{R}^n} |xf(x)|^2 dx \right)^{1/2} \left(\int_{\mathbb{R}^n} |\xi \hat{f}(\xi)|^2 dx \right)^{1/2} \ge \int_{\mathbb{R}^n} |f(x)|^2 dx, \tag{1.3}$$

making a connection between a function and its Fourier Transform as we also mentioned above. In this direction we talk about Hardy's Uncertainty Principle, named after the British mathematician Godfrey H. Hardy who stated,

$$|f(x)| \le Ce^{-\alpha|x|^2}, \quad |\hat{f}(\xi)| \le Ce^{-\beta|\xi|^2}, \quad \alpha\beta > 1/4, \quad \Longrightarrow \quad f \equiv 0.$$
(1.4)

Moreover, if $\alpha\beta = 1/4$ then the function f is a Gaussian, say $f(x) = Ce^{-\alpha|x|^2}$. These functions are precisely the minimizers of the Uncertainty Principle, meaning that equality is only attained for these objects. The proof of this result and its different variants use complex analysis, more concretely the so-called Phragmèn-Lindelöf principle that we will not discuss here.

Hardy's result can be applied on the solution u of (1.1) but on the free particle case, this is, the case where no potential appears. To do so, we need to establish a relation between a function and its Fourier Transform in terms of the solution u and the initial data of the problem u_0 . For this purpose we write an explicit formula for the solution as follows,

$$u(x,t) = e^{it\Delta}u_0(x) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-it|\xi|^2 + ix\cdot\xi} \hat{u}_0(\xi) \,d\xi.$$
(1.5)

Simple computations give that identity (1.5) can also be written as

$$u(x,t) = \frac{1}{(4\pi i t)^{n/2}} \int_{\mathbb{R}^n} e^{i\frac{|x-y|^2}{4t}} u_0(y) \, dy$$
$$= \frac{e^{i\frac{|x|^2}{4t}}}{(4\pi i t)^{n/2}} \int_{\mathbb{R}^n} e^{-i\frac{x}{2t}y} e^{i\frac{|y|^2}{4t}} u_0(y) \, dy.$$

As a consequence

$$e^{it\Delta}u_0(x) = \frac{e^{i|x|^2/4t}}{(2it)^{n/2}}\hat{f}_t\left(\frac{x}{2t}\right),$$
(1.6)

with $f_t(x) = e^{i|x|^2/4t}u_0(x)$. In particular, we can state a version of Hardy's result (1.4) using the connection between u and u_0 , say

If
$$e^{\frac{|x|^2}{\beta^2}}u_0(x)$$
, $e^{\frac{|x|^2}{\alpha^2}}e^{it\Delta}u_0(x) \in L^2(\mathbb{R}^n)$ and $\alpha\beta \le 4t$, then $u_0 \equiv 0$. (1.7)

Identity (1.6) implies that to give size conditions of u at two different times, say t = 0 and t = T is equivalent to give size conditions to f_T and \hat{f}_T . This idea has been largely exploited by L. Escauriaza, C.E. Kenig, G. Ponce, and L. Vega. This type of results give alternative proofs to these classical results using techniques of Partial Differential Equations, more concretely the so-called Carleman type inequalities. These UPs are rigidity results in the sense that the conclusions are that the only function satisfying the desired properties is either the trivial one, or some specific function, as for example the Gaussian in the case of Hardy's UP as we have already seen. Unlike this, the use of Carleman inequalities is rather flexible and allows perturbations by potentials $V \neq 0$.

Another kind of Uncertainty Principle for the Fourier Transform says that if a function $f \in L^1(\mathbb{R}^n)$ is non-zero and has compact support then \hat{f} cannot satisfy a condition of the type $\hat{f}(\xi) = \mathcal{O}(e^{-\epsilon|\xi|})$ for any $\epsilon > 0$. These type of results are named after R. Paley, and N. Wiener. In [51] they give a characterization of a function or distribution with compact support in terms of the analiticity properties of its Fourier Transform.

Following this idea for the solution to the Schrödinger equation we have the following result by C.E. Kenig, G. Ponce and L. Vega that can be found in [7].

Theorem 1.2.1. Let $u \in C([0,1]: L^2(\mathbb{R}^n))$ be a strong solution of the equation

$$\partial_t u = i(\Delta u + V(x,t)u), \quad (x,t) \in \mathbb{R}^n \times [0,1].$$

Assume that

$$\sup_{0 \le t \le 1} \int_{\mathbb{R}^n} |u(x,t)|^2 dx \le A_1,$$
$$\int_{\mathbb{R}^n} e^{2a_1|x_1|} |u(x,0)|^2 dx \le A_2, \quad \text{for some } a_1 > 0,$$
$$\sup_{x \ge 0} u(\cdot,1) \subset \{x \in \mathbb{R}^n : x_1 \le a_2\}$$

for some $a_2 < \infty$ with

$$V \in L^{\infty} \left(\mathbb{R}^n \times [0,1] \right), \quad \|V\|_{L^{\infty}(\mathbb{R}^n \times [0,1])} = M_0$$

and

$$\lim_{\rho \to +\infty} \|V\|_{L^1([0,1]:L^\infty(\mathbb{R}^n \setminus B_\rho))} = 0.$$

Then $u \equiv 0$.

Although we are not going to give the details of the proof of the theorem (see [7]), it is important to point out that they use two important tools that we will be using, namely, Appell's Conformal transformation and Carleman's estimate. The former allows the introduction of parameters α and β via dilations on the

Lower bounds

space and time variables. In this way, we can establish a relation between the rest of the parameters and manipulate them in order to obtain nice bounds. The latter gives us the bounds we are talking about.

Our main purpose is to start to explore the way to reduce the hypothesis from two times to just one. In particular, we look for conditions on u_0 . Besides the fact that we consider this a very natural question by itself, our main motivation has been to try to adapt the PDE techniques to prove more sophisticated UPs. As an example we have the following result by P. Jamming in [30],

Theorem 1.2.2. There exists a constant C such that, for every sets $S, \Sigma \subset \mathbb{R}^d$ of finite Lebesgue measure and for every $f \in L^2(\mathbb{R}^n)$

$$\int_{\mathbb{R}^n} |f(x)|^2 dx \le C e^{C \min\left(|S||\Sigma|, |S|^{1/n} w(\Sigma), w(S)|\Sigma|^{1/n}\right)} \left(\int_{\mathbb{R}^n \setminus S} |f(x)|^2 dx + \int_{\mathbb{R}^n \setminus \Sigma} |\widehat{f}(x)|^2 dx \right)$$

where $w(\Sigma)$ is the mean width of Σ .

This result is an extension to dimension $n \ge 1$ of a result by F. L. Nazarov [52]. Nevertheless we are far from obtaining such results.

1.3 Lower bounds

Up to this point we have focused on the conditions required to conclude that the only solution to the given Schrödinger problem is the trivial solution $u \equiv 0$. Now we are interested on quantifying the solution, i.e. estimating the probability to find the particle described by (1.1). The question is now what requirements do we need in order to do so. The starting point will be the following result:

Theorem 1.3.1. Let $u \in C([0,1] : H^1(\mathbb{R}^n))$ be a strong solution of

$$i\partial_t u + \Delta u + V u = 0, \quad t \in [0, 1], \quad x \in \mathbb{R}^n.$$

If

$$\int_{0}^{1} \int_{\mathbb{R}^{n}} \left(|u|^{2} + |\nabla_{x}u|^{2} \right) (x, t) dx dt \leq A^{2},$$
$$\int_{1/2 - 1/8}^{1/2 + 1/8} \int_{|x| < 1} |u|^{2} (x, t) dx dt \geq 1,$$

and

$$\|V\|_{L^{\infty}(\mathbb{R}^n \times [0,1])} \le L,$$
 (1.8)

then there exists $R_0 = R_0(n, A, L) > 0$ and a constant c = c(n) such that for $R \ge R_0$ it follows that

$$\delta(R) \equiv \left(\int_0^1 \int_{R-1 < |x| < R} \left(|u|^2 + |\nabla_x u|^2 \right) (x, t) dx dt \right)^{1/2} \ge c e^{-cR^2}.$$
 (1.9)

We see that the main assumption is that the L^2 norm of u is bounded from below in a small time-space cylinder around the origin. Since we are looking for conditions on u_0 it is only natural to wonder if there exist conditions that imply this hypothesis. This will be the topic of chapter 3.

The key point to prove Theorem 1.3.1 is the use of Carleman estimates. These estimates allow us to find lower bounds for suitable functions.

Lemma 1.3.2 Carleman estimate. Assume that R > 0 and $\varphi : [0,1] \longrightarrow \mathbb{R}$ is a smooth function. Then, there exists $\hat{c_n} = c(n, \| \varphi' \|_{\infty} + \| \varphi'' \|_{\infty}) > 0$ such that the inequality

$$\frac{\sigma^{3/2}}{\hat{c_n}R^2} \parallel e^{\sigma \left|\frac{x}{R} + \varphi(t)e_1\right|^2} g \parallel_2 \leq \parallel e^{\sigma \left|\frac{x}{R} + \varphi(t)e_1\right|^2} (i\partial_t + \Delta)g \parallel_2, \tag{1.10}$$

holds when $\sigma \geq \hat{c_n} R^2$ and $g \in \mathcal{C}_0^{\infty}(\mathbb{R}^{n+1})$ has its support contained in the set

$$\left\{ (x,t) : \left| \frac{x}{R} + \varphi(t)e_1 \right| \ge 1 \right\}.$$

Proof. Let $f = e^{\sigma |\frac{x}{R} + \varphi(t)e_1|^2}g$. Then,

$$e^{\sigma \left|\frac{x}{R} + \varphi(t)e_1\right|^2} (i\partial_t + \Delta)g = S_{\sigma}f - 4\sigma A_{\alpha}f,$$

where

$$S_{\sigma} = i\partial_t + \Delta + \frac{4\sigma^2}{R^2} |\frac{x}{R} + \varphi(t)e_1|^2,$$
$$A_{\sigma} = \frac{1}{R} (\frac{x}{R} + \varphi(t)e_1) \cdot \nabla + \frac{n}{2R^2} + \frac{i\varphi'}{2} (\frac{x_1}{R} + \varphi),$$

are the symmetric and anti-symmetric operators respectively. Thus,

$$A^*_{\sigma} = -A_{\sigma}, \qquad S^*_{\sigma} = S_{\sigma}$$

and

$$\| e^{\sigma \left| \frac{x}{R} + \varphi(t) e_1 \right|^2} (i\partial_t + \Delta) g \|_2^2 = \langle S_\sigma f - 4\sigma A_\sigma f, S_\sigma f - 4\sigma A_\sigma f \rangle$$

$$\geq -4\sigma \langle (S_\sigma A_\sigma - A_\sigma S_\sigma) f, f \rangle = -4\sigma \langle [S_\sigma, A_\sigma] f, f \rangle.$$

A calculation shows that

$$[S_{\sigma}, A_{\sigma}] = \frac{2}{R^2} \Delta - \frac{4\sigma^2}{R^4} \left| \frac{x}{R} + \varphi(t)e_1 \right|^2 - \frac{1}{2} \left[\left(\frac{x_1}{R} + \varphi(t) \right) \varphi'' + \varphi'^2 \right] + \frac{2i\varphi'}{R} \partial_{x_1},$$

and

$$\| e^{\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} (i\partial_t + \Delta)g \|_2^2 \ge \frac{16\sigma^3}{R^4} \int \left| \frac{x}{R} + \varphi e_1 \right|^2 |f|^2 dx dt + \frac{8\sigma}{R^2} \int |\nabla f|^2 dx dt$$

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$$+2\sigma \int \left[\left(\frac{x_1}{R}+\varphi\right)\varphi''+\varphi'^2\right]|f|^2dxdt-\frac{8\sigma i}{R}\int \varphi'(\partial_{x_1}f)fdxdt.$$

Hence using the hypothesis on the support of g and the Cauchy-Schwarz inequality, the absolute value of the last two terms can be bounded by a fraction of the first two terms on the right hand side when $\sigma \geq \hat{c_n}R^2$ for some large $\hat{c_n}$ depending on the dimension and $\|\varphi'\|_{\infty} + \|\varphi''\|_{\infty}$. Then the result follows.

The proof of Theorem 1.4.1 follows the same strategy as the one for Theorem 1.3.1. The only thing we introduce is Appell's Conformal transformation. This result allows us define a new family of solutions depending on certain parameters. The lemma is the following,

Lemma 1.3.3. If u(y,s) verifies

$$\partial_s u = i(\Delta u + V(y, s)u + F(y, s)), \quad (y, s) \in \mathbb{R}^n \times [0, 1]$$

and α and β are positive, then

$$\tilde{u}(x,t) = \left(\frac{\sqrt{\alpha\beta}}{\alpha(1-t) + \beta t}\right)^{n/2} u\left(\frac{\sqrt{\alpha\beta}x}{\alpha(1-t) + \beta t}, \frac{\beta t}{\alpha(1-t) + \beta t}\right) e^{\frac{(\alpha-\beta)|x|^2}{4i(\alpha(1-t) + \beta t)}}$$

verifies

$$\partial_t \tilde{u} = i(\Delta \tilde{u} + \tilde{V}(x,t)\tilde{u} + \tilde{F}(x,t)), \quad (x,t) \in \mathbb{R}^n \times [0,1]$$

with

$$\tilde{V}(x,t) = \frac{\alpha\beta}{(\alpha(1-t)+\beta t)^2} V\left(\frac{\sqrt{\alpha\beta}x}{\alpha(1-t)+\beta t}, \ \frac{\beta t}{\alpha(1-t)+\beta t}\right)$$

and

$$\tilde{F}(x,t) = \left(\frac{\sqrt{\alpha\beta}}{\alpha(1-t)+\beta t}\right)^{n/2+2} F\left(\frac{\sqrt{\alpha\beta}x}{\alpha(1-t)+\beta t}, \frac{\beta t}{\alpha(1-t)+\beta t}\right) e^{\frac{(\alpha-\beta)|x|^2}{4i(\alpha(1-t)+\beta t)}}.$$

Although the statement uses two parameters α and β we are going to define $\gamma = \alpha/\beta$ and rewrite the dilations in a proper way. We need to be careful on how these functions alter the domains of integration in the proof. It is important to make a sensible use of the parameter γ in relation to these functions. For this reason, we give some estimations in the next section. We will not be considering the function F either, since we will not consider outer forces disturbing our system.

1.4 The main results

By $\mathcal{H}^1_{loc}(\mathbb{R}^n)$ we mean the set of functions f that together with their gradients are locally in $L^2(\mathbb{R}^n)$. We have the following result.

Theorem 1.4.1. Let $u \in \mathcal{C}([0,1] : \mathcal{H}^1_{loc}(\mathbb{R}^n))$ be a solution of

$$\begin{cases} \partial_t u = i(\Delta u + V(x, t)u) \\ u(x, 0) = u_0(x), \end{cases}$$

where $V \in L^{\infty}(\mathbb{R}^n \times [0,1])$ is a complex potential and

$$\parallel V \parallel_{L^{\infty}(\mathbb{R}^n \times [0,1])} \leq L.$$

Let $R_0 > 0$ be such that for some $c_0 > 0$,

$$\int_{B_{R_0}} |u_0|^2 dx = c_0^2, \tag{1.11}$$

and let also $M \ge 4R_0 + 1$ so that

$$\sup_{0 \le t \le 1} \int_{B_M} |u(x,t)|^2 + |\nabla u(x,t)|^2 dx = A^2 < +\infty.$$
(1.12)

Then, there exist $t^* = \min\left(\frac{256A}{c_0L}, 2^{-14}\left(\frac{c_0}{A}\right)^4, R_0^2, \frac{1}{L^2}\right)$ and a universal constant c_n that depends just on the dimension such that if $0 < t < t^*$,

$$\frac{e^{c_n \frac{\rho^2}{t}}}{t} \int_{t/4}^{3t} \int_{||y|-\rho-\rho\frac{s}{t}|<4\rho\sqrt{t}} |u(y,s)|^2 + s|\nabla_y u(y,s)|^2 \, dyds \ge c_0^2, \qquad R_0 \le \rho \le M.$$
(1.13)

Remark: Observe that M can be infinite.

Our second main result is an immediate consequence of Theorem 1.4.1, and therefore the proof will be omitted. As far as we know this type of uniqueness result is completely new.

Theorem 1.4.2. Assume that for any $u_0 \in H^1(\mathbb{R}^n)$ there exists a unique solution $u \in \mathcal{C}([0,1] : H^1(\mathbb{R}^n))$ of

$$\begin{cases} \partial_t u = i \left(\Delta + V(x, t) \right) u \quad x \in \mathbb{R}^n, \quad t \in (0, 1) \\ u(x, 0) = u_0, \end{cases}$$

with $V \in L^{\infty}(\mathbb{R}^n \times [0,1])$. If c_n is as in (1.13) and there exist $R_j, R_j \to \infty, j \in \mathbb{N}$ such that for all j

$$\lim_{t \downarrow 0} \frac{1}{t} e^{c_n \frac{R_j^2}{t}} \int_{t/4}^{3t} \int_{||y| - R_j(1+s/t)| < 4R_j\sqrt{t}} |u(y,s)|^2 + s |\nabla u(y,s)|^2 \, dy \, ds = 0,$$

then $u \equiv 0$.

Some a priori estimates

As a side result to Theorem 1.4.2 we could let the spatial parameter ρ tends to infinity and obtain a similar conclusion.

Theorem 1.4.3. Assuming the same conditions as in Theorem 1.4.2 and that there exists $t_0 < t^*$ such that

$$\lim_{\rho \to \infty} \frac{1}{t_0} e^{c_n \frac{\rho^2}{t_0}} \int_{t_0/4}^{3t_0} \int_{||y| - \rho(1 + s/t_0)| < 4\rho\sqrt{t_0}} |u(y, s)|^2 + s |\nabla u(y, s)|^2 \, dy \, ds = 0,$$

then $u \equiv 0$.

Remark: Notice that our results are perturbative and allow complex potentials that can depend on time. Therefore, it can be applied to solutions of non-linear equations as long as a nice local in time well-posedness theory is available. We can proceed as done in [6] and consider for example

$$\partial_t u = i(\Delta u + f(|u|^2)u), \tag{1.14}$$

with $f : \mathbb{R} \to \mathbb{R}$, and f(0) = f'(0) = 0. Then, given two smooth solutions u_1 and u_2 of (1.14), the difference $\omega = u_1 - u_2$ satisfies an equation as (1.1), and therefore Theorems 1.4.2 and 1.4.3 apply to ω .

1.5 Some a priori estimates

Before going into the proof of the theorem, we give some estimates of the support functions we are going to be using. At some point in the previous section we have talked about Appell's conformal transformation and mentioned that the parameters α and β will be replaced by $\gamma > 0$ defined as the relation between the former ones, say α/β . We will also want this parameter γ to be as big as possible so in principle we see it as $\gamma >> 1$. Having this in mind, we define the following functions:

$$\alpha(t) = \frac{1}{\gamma^{1/2}(1-t) + \gamma^{-1/2}t},$$
(1.15)

$$s(t) = \frac{t}{\gamma(1-t)+t},$$
 (1.16)

$$\beta(t) = \frac{1}{1 - t + \gamma^{-1}t} - \frac{1}{\gamma(1 - t) + t}.$$
(1.17)

At some point on the proof there will be a change of variables so it is interesting to see how we can write t in terms of s and see how the measure changes with respect to γ . First we see that

$$t(s) = \frac{s\gamma}{1+s(\gamma-1)},$$
 (1.18)

and so

$$dt = \frac{\gamma}{(1 + s(\gamma - 1))^2} ds.$$

Along the proof we encounter two different time intervals due to the definition of the cut-off functions. The first one is [3/8, 5/8]. For this interval observe that $\alpha(t)$ can be estimated by

$$\frac{1}{\gamma^{1/2}} \le \alpha(t) \le \frac{3}{\gamma^{1/2}},$$
 (1.19)

and the variable s lives in

$$I_s^1 = \left[\frac{3}{5\gamma + 3}, \frac{5}{3\gamma + 5}\right].$$
 (1.20)

The length of this interval can be estimated by

$$\frac{1}{4\gamma} \le |I_s^1| \le \frac{2}{\gamma},\tag{1.21}$$

and the differential,

$$\frac{\gamma}{8}ds \le dt \le \gamma ds. \tag{1.22}$$

On the other hand, when $t \in [1/4, 3/4]$ we can make the following estimations:

$$\frac{1}{\gamma^{1/2}} \le \alpha(t) \le \frac{4}{\gamma^{1/2}},\tag{1.23}$$

$$0 \le \beta(t) = \frac{1}{1 - t + \gamma^{-1}t} - \frac{1}{\gamma(1 - t) + t} \le \frac{1}{1 - t + \gamma^{-1}t} \le 4.$$
(1.24)

It should also be noticed that the variable s lives on the interval

$$I_s^2 = \left[\frac{1}{3\gamma+1}, \frac{3}{\gamma+3}\right],\,$$

and its length is bounded from above and below as follows

$$\frac{1}{2\gamma} \le |I_s^2| \le \frac{3}{\gamma},\tag{1.25}$$

which means that when γ is large the variable s has size γ^{-1} and so we have the following estimation for the differential

$$\frac{\gamma}{16}ds \le dt \le \gamma ds. \tag{1.26}$$

Observe next that if we combine (1.15) with (1.18) we can write

$$\sqrt{\gamma}\alpha(t(s)) = 1 + s\gamma - s. \tag{1.27}$$

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Proof of Theorem 1.4.1

Assume now that $u \in \mathcal{C}([0,1], \mathcal{H}^1_{loc}(\mathbb{R}^n))$ is a solution to (1.1). Then, the following identity holds

$$|u(x,t)|^{2} - |u(x,0)|^{2} = -2Im \int_{0}^{t} \left(div(u(x,s) \cdot \nabla \overline{u}(x,s)) + V(x,s)|u(x,s)|^{2} \right) ds,$$
(1.28)

where V is a complex bounded potential. The proof of this identity is the following:

First observe that

$$div(u\nabla\bar{u}) = |\nabla u|^2 + u\Delta\bar{u} \Rightarrow u\Delta\bar{u} = div(u\nabla\bar{u}) - |\nabla u|^2,$$

and so we compute the derivative on the second variable of the squared term

$$\begin{split} \frac{d}{dt}|u(x,t)|^2 &= \frac{d}{dt}(u\bar{u}) = \partial_t u\bar{u} + u\partial_t \bar{u} \\ &= \overline{u\partial_t \bar{u}} + u\partial_t \bar{u} = 2Re(u\partial_t \bar{u}) \\ &= 2Re(ui(\Delta + V)\bar{u}) = 2Re(iu\Delta\bar{u} + iV|u|^2) \\ &= -2Im(u\Delta\bar{u} + V|u|^2) \\ &= -2Im(div(u\nabla\bar{u}) - |\nabla u|^2 + V|u|^2) \\ &= -2Im(div(u\nabla\bar{u}) + V|u|^2), \end{split}$$

which concludes the proof.

We are ready now to discuss the proof of the main theorem on this chapter.

1.6 Proof of Theorem 1.4.1

We follow very closely the arguments in [7]. The goal is to use the Carleman estimate (1.10) in a suitable way so that we can control both u and ∇u by the initial data. For this purpose we want to build an auxilliary function g. First, let γ be large enough, say $\gamma > 16$ and define $R = R_0 \sqrt{\gamma}$. Define also the following cut-off functions, $\theta_R, \eta \in \mathcal{C}_0^{\infty}(\mathbb{R}^n), \varphi \in \mathcal{C}^{\infty}([0, 1])$

$$\theta_R(x) = \begin{cases} 1, & |x| \le R \\ 0, & |x| \ge R+1, \end{cases} \quad \eta(x) = \begin{cases} 1, & |x| \ge 2 \\ 0, & |x| \le 3/2, \end{cases}$$
(1.29)

$$\varphi(t) = \begin{cases} 4, & t \in [3/8, 5/8] \\ 0, & t \in [0, 1/4] \cup [3/4, 1]. \end{cases}$$

For future purposes we will be assuming that $R \geq 2$. Next we use the Appell Conformal transformation (1.3.3) on the solution u to generate a new family of solutions depending on the parameter γ , say

$$v(x,t) = \alpha(t)^{n/2} u(\alpha(t)x, s(t)) e^{-\frac{i}{4}\beta(t)|x|^2} \quad , \quad (x,t) \in \mathbb{R}^n \times [0,1],$$

where the functions α , β and s were introduced on the previous section.

We use all the information gathered above to define the function q as follows:

$$g(x,t) = \theta_R(x)\eta\left(\frac{x}{R} + \varphi(t)e_1\right)v(x,t) \quad , \quad (x,t) \in \mathbb{R}^n \times [0,1].$$

Observe that due to the nature of the test functions, g is compactly supported and.

- $g = \theta_R v$ on $(x,t) \in \{|x| \le R+1\} \times [3/8, 5/8],$ $\nabla_x v(x,t) = \alpha(t)^{n/2} e^{-\frac{i}{4}\beta(t)|x|^2} (\alpha(t)\nabla u \frac{i}{2}\beta(t)x \cdot u),$
- supp $g \subseteq \{ \left| \frac{x}{R} + \varphi e_1 \right| \ge 1 \}$, where $u = u(\alpha(t)x, s(t))$.

With the function we just defined, we are ready to use the Carleman estimate. Recall that for $\sigma \geq \hat{c_n} R^2$

$$\frac{\sigma^{3/2}}{\hat{c}_n R^2} \| e^{\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} g(x,t) \|_2 \le \| e^{\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} (i\partial_t + \Delta)g(x,t) \|_2 .$$
(1.30)

We need to work out both sides of the inequality. The goal is to give an estimation from below to the left hand side using the information we have about the initial data. Once this is done, we will find suitable upper estimates of the right hand side in order to absorb the terms we do not need using the parameter σ . Let's thus look at the l.h.s. of the inequality above,

$$\begin{split} \| e^{\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} g(x,t) \|_2^2 &= \int_t \int_x e^{2\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} |g(x,t)|^2 dx dt \\ &\geq e^{8\sigma} \int_{3/8}^{5/8} \int_{|x| \le R+1} |\theta_R(x)v(x,t)|^2 dx dt \\ &= e^{8\sigma} \int_{3/8}^{5/8} \int_{|x| \le R+1} \alpha(t)^n |\theta_R(x)u(\alpha(t)x,s(t))|^2 dx dt \\ &\geq e^{8\sigma} \frac{\gamma}{8} \int_{s(\frac{3}{5})}^{s(\frac{5}{3})} \int_{|y| \le \alpha(t(s))(R+1)} |\theta_R(\alpha^{-1}(t(s))y)u(y,s)|^2 dy ds. \end{split}$$

We have made the change of variables $y = \alpha(t)x$ and s = s(t) together with the estimate (1.22) on the differential and change of measure we mentioned on the previous section. Now we want to plug the initial data into the equation. To do so we measure the size of the difference between our function u and the initial data u_0 , say

$$B = \left| \int_{s \sim \gamma^{-1}} \int_{|y| \le \alpha(t(s))R} \theta_R^2(\alpha^{-1}(t(s))y)(|u|^2 - |u_0|^2) dy ds \right|.$$

Next we use (1.28) to obtain,

$$\begin{split} B &= \left| \int_{s \sim \gamma^{-1}} \int_{y} \theta_{R}^{2} \left(-2Im \int_{0}^{s} (div(u\nabla\bar{u}) + V|u|^{2}) ds' \right) dy ds \right| \\ &= \left| 2Im \int_{s \sim \gamma^{-1}} \int_{0}^{s} \int_{y} \theta_{R}^{2} (div(u\nabla\bar{u}) + V|u|^{2}) dy ds' ds \right| \\ &\leq \left| 2Im \int_{s} \int_{s'} \int_{y} \theta_{R}^{2} div(u\nabla\bar{u}) dy ds' ds \right| + \left| 2Im \int_{s} \int_{s'} \int_{y} \theta_{R}^{2} V|u|^{2} dy ds' ds \right| \\ &= B_{1} + B_{2}. \end{split}$$

Here we study the contribution of both integrals separately and see how to choose γ in a suitable way depending on the parameters c_0 , A and L so that we have a nice bound from below for the left hand side of Carleman's estimate on this particular case. For the estimation of both B_1 and B_2 we use (1.21), (1.22) and (1.12) so that

$$B_{2} = \left| 2Im \int_{s} \int_{s'} \int_{y} \theta_{R}^{2}(\alpha^{-1}(t(s)))V(y,s')|u(y,s')|^{2}dyds'ds \right|$$

$$\leq \frac{4L}{\gamma} \int_{s'} \int_{y} |u|^{2}dyds'$$

$$\leq \frac{8L}{\gamma^{2}} \sup_{s' \sim \gamma^{-1}} \int_{|y| \leq 4R/\sqrt{\gamma}} |u|^{2}dy$$

$$\leq \frac{8A^{2}L}{\gamma^{2}}.$$

As for B_1 we have, using integration by parts,

$$\begin{split} B_{1} &= \left| 4Im \int_{s \sim \gamma^{-1}} \int_{0}^{s} \alpha^{-1}(t(s)) \int_{|y| \leq \alpha(t(s))R} (\theta_{R} \nabla \theta_{R})(u \nabla \bar{u}) dy ds' ds \right| \\ &\leq \left| 4\sqrt{\gamma} Im \int_{s \sim \gamma^{-1}} \int_{s' \sim \gamma^{-1}} \int_{y} (\theta_{R} \nabla \theta_{R})(u \nabla \bar{u}) dy ds' ds \right| \\ &\leq 4\sqrt{\gamma} \int_{s \sim \gamma^{-1}} \int_{s' \sim \gamma^{-1}} \int_{y} |u \nabla \bar{u}| dy ds' ds \\ &\leq 16\gamma^{-3/2} \sup_{s' \sim \gamma^{-1}} \int_{|y| \leq \alpha(t(s))R} |u \nabla \bar{u}| dy \\ &\leq 8\gamma^{-3/2} \sup_{s' \sim \gamma^{-1}} \int_{|y| \leq 4R/\sqrt{\gamma}} |u|^{2} + |\nabla u|^{2} dy \\ &\leq \frac{8A^{2}}{\gamma^{3/2}}. \end{split}$$

Now if we put all together and remember that there was a factor γ multiplying the equation, we have

$$\gamma B \le \frac{8A^2}{\gamma^{1/2}} + \frac{8A^2L}{\gamma} = \frac{8A^2}{\gamma^{1/2}}(1 + L\gamma^{-1/2}).$$

Therefore, if we choose $\gamma \geq L^2$ we have that

$$\gamma B \le \frac{16A^2}{\gamma^{1/2}}.$$

Now we want to hide the contribution of B using c_0 . To do so we need to work out the extra term introduced when B was defined, say

$$\gamma \int_s \int_y \theta_R^2(\alpha^{-1}(t(s))y) |u_0|^2 dy ds.$$

Clearly, the inclusion $B_{\alpha(t(s))R} \subset B_{\alpha(t(s))(R+1)}$ and the definition of θ_R together with (1.21) and (1.11) gives us

$$\begin{split} \gamma \int_{s} \int_{B_{\alpha(t(s))(R+1)}} \theta_{R}^{2} |u_{0}|^{2} dy ds &\geq \gamma \int_{s} \int_{B_{\alpha(t(s))R}} \theta_{R}^{2} |u_{0}|^{2} dy ds \\ &= \gamma \int_{s} \int_{B_{\alpha(t(s))R}} |u_{0}|^{2} dy ds \\ &\geq \gamma \frac{1}{4\gamma} \int_{B_{R_{0}}} |u_{0}|^{2} dy \\ &\geq \frac{c_{0}^{2}}{4}. \end{split}$$

Proof of Theorem 1.4.1

Thus if $\frac{c_0^2}{8} \ge 16A^2\gamma^{-1/2}$, then

$$\gamma \ge 2^{14} \left(\frac{A}{c_0}\right)^4,$$

and we can hide the contribution of B inside c_0^2 and conclude

$$\| e^{\sigma \left| \frac{x}{R} + \varphi(t) e_1 \right|^2} g(x, t) \|_2^2 \ge \frac{e^{8\sigma}}{64} c_0^2.$$
(1.31)

Now we study the right hand side of the Carleman estimate. First compute the operator to see how the supports of the resulting expressions change:

$$(i\partial_t + \Delta)g(x,t) = \theta_R \eta \bar{V}v + \theta_R (i\varphi'\partial_{x_1}\eta v + 2R^{-1}\nabla\eta \cdot \nabla v + R^{-2}\Delta\eta v) + \eta (2\nabla\theta_R \cdot \nabla v + \Delta\theta_R v) = E_1 + E_2 + E_3,$$

where E_2 and E_3 are supported in • $3/2 \le \left|\frac{x}{R} + \varphi(t)\right| \le 2$, $t \in [1/4, 3/4]$,

• $\{R \le |x| \le R+1\} \times [1/4, 3/4]$ respectively. From the definition of the conformal transformation and the assumption on V we have that $|\tilde{V}| \leq L\gamma^{-1}$ on the support of g. Thus,

$$\begin{split} \parallel e^{\sigma \left|\frac{x}{R} + \varphi(t)e_{1}\right|^{2}} (i\partial_{t} + \Delta)g(x,t) \parallel_{2}^{2} &= \int_{t} \int_{x} e^{2\sigma \left|\frac{x}{R} + \varphi(t)e_{1}\right|^{2}} |(i\partial_{t} + \Delta)g(x,t)|^{2} dx dt \\ &\leq L^{2}\gamma^{-2} \parallel e^{\sigma \left|\frac{x}{R} + \varphi(t)e_{1}\right|^{2}}g \parallel_{2}^{2} \\ &+ e^{8\sigma} \int_{1/4}^{3/4} \int_{|x| \le R+1} (|v|^{2} + 4R^{-2}|\nabla v|^{2}) dx dt \\ &+ e^{72\sigma} \int_{1/4}^{3/4} \int_{R \le |x| \le R+1} (|v|^{2} + |\nabla v|^{2}) dx dt \\ &= L^{2}\gamma^{-2} \parallel e^{\sigma \left|\frac{x}{R} + \varphi(t)e_{1}\right|^{2}}g \parallel_{2}^{2} + e^{8\sigma}I_{1} + e^{72\sigma}I_{2}. \end{split}$$

Observe that from (1.30) the first term can be absorbed by the left hand side of the inequality if

$$\frac{\sigma^{3/2}}{c_n R^2} \ge \frac{2L}{\gamma}.\tag{1.32}$$

So we only need to study the contribution of I_1 and I_2 . To see things more clearly we split I_1 in the sub-integrals I_{11} , I_{12} , the first one measuring the contribution of v, and the second one doing the same for the gradient ∇v .

$$I_{11} = \int_{1/4}^{3/4} \int_{|x| \le R+1} |v|^2 dx dt = \int_{1/4}^{3/4} \int_{|x| \le R+1} \alpha(t)^n |u(\alpha(t)x, s(t))|^2 dx dt$$
$$\leq \gamma \int_{s(1/4)}^{s(3/4)} \int_{|y| \le \alpha(t(s))(R+1)} |u(y, s)|^2 dy ds.$$

Here we have simply made a change of variables and use the information we have about the behavior of the functions $\alpha(t)$ and s(t) when γ is large enough. As for I_{12} we use the triangular inequality together with the change of variables $y = \alpha(t)x$ and the estimations with γ , as we see here

$$\begin{split} I_{12} &= \int_{1/4}^{3/4} \int_{|x| \le R+1} 4R^{-2} |\nabla v|^2 dx dt \\ &= 4R^{-2} \int_{1/4}^{3/4} \int_{|x| \le R+1} \alpha(t)^n |\alpha(t) \nabla u - \frac{i}{2} \beta(t) x u|^2 dx dt \\ &\le 4R^{-2} \gamma \int_{s(1/4)}^{s(3/4)} \int_{|y| \le \alpha(t(s))(R+1)} |\alpha(t(s)) \nabla u(y,s) - \frac{i}{2} \beta(t(s)) \alpha^{-1}(t(s)) y u|^2 dy ds \\ &\le 4R^{-2} \gamma \int_{s\sim 1/\gamma} \int_{|y| \le \alpha(t(s))(R+1)} \left(\frac{16}{\gamma} |\nabla u|^2 + 4(R+1)^2 |u|^2\right) dy ds \\ &= 4\gamma \int_{s\sim 1/\gamma} \int_{|y| \le \alpha(t(s))(R+1)} \left(\frac{16}{R^2 \gamma} |\nabla u|^2 + 4\left(1 + \frac{1}{R}\right)^2 |u|^2\right) dy ds. \end{split}$$

Using now that $R = R_0 \sqrt{\gamma} \ge 2$ we get

$$I_{12} \le 36\gamma \int_{s \sim \gamma^{-1}} \int_{|y| \le \alpha(t(s))(R+1)} |u|^2 + \gamma^{-1} |\nabla u|^2 dy ds.$$

And if we put both I_{11} and I_{12} together and use (1.25) we can estimate I_1 as follows

$$I_{1} \leq 72\gamma \int_{s \sim \frac{1}{\gamma}} \int_{|y| \leq \alpha(t(s))(R+1)} (|u|^{2} + \gamma^{-1} |\nabla u|^{2}) dy ds$$
(1.33)

$$\leq 216 \sup_{s \sim \gamma^{-1}} \int_{|y| \leq \alpha(t(s))(R+1)} (|u|^2 + \gamma^{-1} |\nabla u|^2) dy$$
(1.34)

$$\leq 216 \sup_{s \sim \gamma^{-1}} \int_{|y| \leq M} (|u|^2 + \gamma^{-1} |\nabla u|^2) dy$$
(1.35)

$$\leq 216A^2$$
. (1.36)

Following a similar computation we can estimate I_2 as,

$$I_2 \le 32\gamma^2 R_0^2 \int_{s \sim \frac{1}{\gamma}} \int_{\alpha(t(s))R \le |y| \le \alpha(t(s))(R+1)} |u|^2 + \gamma^{-1} |\nabla u|^2 dy ds.$$

Observe now that the spatial variable y lives in a region of length α . We would like to rewrite that region in terms of γ . Using (1.23) and (1.27) together with an appropriate estimation for s we have that I_2 can be written as

$$I_2 \le \gamma^2 32R_0^2 \int_{s \sim \gamma^{-1}} \int_{||y| - R_0 - R_0 s\gamma| < \frac{4R_0}{\sqrt{\gamma}}} |u|^2 + \gamma^{-1} |\nabla u|^2 dy ds.$$

Now if we put everything together we have the following inequality

$$\frac{\sigma^{3/2}}{\hat{c_n}R^2} \frac{c_0}{16} \le 16A + 6\gamma R_0 e^{36\sigma} \left(\int_{s \sim \gamma^{-1}} \int_{||y| - R_0 - R_0 s\gamma| < \frac{4R_0}{\sqrt{\gamma}}} (|u|^2 + \gamma^{-1} |\nabla u|^2) dy ds \right)^{1/2}.$$
(1.37)

To hide the first term of the right hand side inside the left hand side we ask the following

$$\frac{\sigma^{3/2}}{\hat{c_n}R^2} \ge \frac{512A}{c_0} \Longrightarrow \sigma \ge c_n R^{4/3},\tag{1.38}$$

for some universal c_n that depends on $\hat{c_n}$, c_0 and A.

Since we want (1.32) and (1.38) to be satisfied we impose the following condition on the parameter γ

$$\frac{2L}{\gamma} \le \frac{512A}{c_0} \Longrightarrow \gamma \ge \frac{c_0 L}{256A}.$$
(1.39)

And thus, whenever

$$\gamma \ge \max\left(\frac{c_0L}{256A}, 2^{14}\left(\frac{A}{c_0}\right)^4, \frac{1}{R_0^2}, L^2\right),$$

we can hide the contribution of the first term on the right hand side of (1.37) into the left hand side, so

$$\frac{\sigma^{3/2}}{\hat{c_n}R^2}\frac{c_0}{32} \le 16R_0\gamma e^{36\sigma} \left(\int_{s\sim\gamma^{-1}}\int_{||y|-R_0-R_0s\gamma|<\frac{4R_0}{\sqrt{\gamma}}}(|u|^2+\gamma^{-1}|\nabla u|^2)dyds\right)^{1/2}.$$

On the other hand σ has to be greater than $\hat{c}_n R^2$ according to Carleman's estimate, which is a stronger condition than the one we just found. Hence if $\sigma = 64\hat{c}_n R^2$ we have that for some universal constant $c_{n,1}$ which depends only on \hat{c}_n ,

$$c_0 \le \left(\gamma e^{c_{n,1}R_0^2\gamma} \int_{s \sim \gamma^{-1}} \int_{||y| - R_0 - R_0 s\gamma| < \frac{4R_0}{\sqrt{\gamma}}} (|u|^2 + s|\nabla u|^2) dy ds\right)^{1/2},$$

now if we rename $\gamma^{-1} \equiv t$ observe that

$$t \le \min\left(\frac{256A}{c_0L}, \ 2^{-14}\left(\frac{c_0}{A}\right)^4, \ R_0^2, \ \frac{1}{L^2}\right) = t^*,$$

and

$$c_0^2 \leq \frac{e^{c_{n,1}\frac{R_0^2}{t}}}{t} \int_{t/4}^{3t} \int_{||y|-R_0-R_0\frac{s}{t}| < 4R_0\sqrt{t}} (|u|^2 + s|\nabla u|^2) dy ds,$$

as we wanted to see.

On the statement of the theorem we write c_n for simplicity. Observe also that if we take $\rho \in [R_0, M]$ the result will still be true. This happens because no matter what ρ we choose, c_0 does not change.

1.7 Some remarks in the periodic case

In this section we explore some consequences of Theorem 1.4.1, in particular on the 1-dimensional periodic case, to see its relation to observability results.

The outcome of Theorem 1.4.1 was that we could give a lower bound to the \mathcal{H}^1 norm of the solution u in a particular region of space. We call this the observability region. Consider the following problem:

$$\begin{cases} i\partial_t u + \Delta u = 0, & \text{in } \Omega \times \mathbb{R}_t, \\ u = 0, & \text{on } \partial\Omega \times \mathbb{R}_t, \\ u(\cdot, 0) = u_0, & \text{in } \Omega, \end{cases}$$
(1.40)

where Ω is a bounded domain of \mathbb{R}^n with a smooth boundary $\partial\Omega$. Observe that this is a local problem and the solution vanishes on the boundary, (which is not our case). Nevertheless it can be proved that u satisfies the following condition:

$$\forall \varepsilon > 0, \quad \forall u_0 \in L^2(\Omega), \quad \|u_0\|_{L^2(\Omega)} \le \mathcal{C}(\varepsilon) \|u\|_{L^2(\omega \times (0,\varepsilon))}, \tag{1.41}$$

 ω being a nonempty open subset of Ω . These type of results are known as observability results and allow us to have some control on u only by having information of the initial data u_0 . Although (1.13) is not an observability result *per se*, it has some similarities to it. The main drawback is that the term of the gradient appears in (1.13) and it is a natural question whether this term is needed. Nonetheless, this term comes multiplied by a time factor which can be very small as t becomes small.

It should also be pointed out that whereas in (1.41) all the information carried by u lies within Ω , in (1.13) the observability region may lie outside the ball B_{R_0} where the information of the initial data is contained.

The region has the particularity that it is dynamic in the sense that it changes in time for certain fixed ρ_0 . On the other hand, for a fixed time t_0 it also changes its geometry if we move the parameter ρ . Recall its definition

$$\left||y| - \rho - \rho \frac{s}{t}\right| < 4\rho\sqrt{t}.$$
(1.42)

Some remarks in the periodic case

The first thing it should be noticed is that the region describes a bounded area on the y-s space-time variables. For simplicity we are going to assume first that we are on dimension 1, i.e. $y \in \mathbb{R}$. The shape of this region will vary with respect to parameters t and ρ .

We will see what happens when t tends to zero but first we look at the other parameter. Unlike t, ρ can be large. Its real size will depend on R_0 , this is, the region where we look at the initial data u_0 .

First we would like to see what the region looks like. Considering $s \in [t/4, 3t]$ observe that:

1. If $s = \frac{t}{4}$ then,

$$\left||y| - \frac{5}{4}\rho\right| < 4\rho\sqrt{t}$$

which is a straight line of centers $-5\rho/4$ and $5\rho/4$ respectively to each side of the space variable and length $8\rho\sqrt{t}$.

2. If s = 3t then,

$$|y| - 4\rho| < 4\rho\sqrt{t}$$

which is a straight line of centers -4ρ and 4ρ and length $8\rho\sqrt{t}$.

Clearly for each $s \in [t/4, 3t]$ we describe a line of length $8\rho\sqrt{t}$ that moves to the right as s grows for y > 0 and to the left if y < 0.

If we sketch it out we would see something like:



Now we play a bit with the geometry of the region. No need to say it is absolutely symmetric with respect to the axis y = 0. The length of the horizontal line between either of the vertices on the same side is $11\rho/4$ and the vertical distance 11t/4 from where we easily calculate the length of the side lines

$$d=\frac{11}{4}\sqrt{t^2+\rho^2}$$

To finish with the small analysis observe that the inclination or slope of the side lines is t/ρ .

A question now arises: does it come across y = 0? In other words, do both symmetric parts meet for some value of the parameters t or ρ ? The answer is no. Consider the closest vertice to y = 0 on the region y > 0. This point is

$$P = \frac{5\rho}{4} - 4\rho\sqrt{t}$$

Assume now that P < 0, $\rho > 0$ and see what happens:

$$P = \frac{5\rho}{4} - 4\rho\sqrt{t} < 0 \Longrightarrow \frac{5}{4} - 4\sqrt{t} < 0$$
$$\Longrightarrow \frac{5}{16} < \sqrt{t} \Longrightarrow t > \frac{25}{256}$$

which is not possible since t has to be smaller than that by definition and hence P > 0. Thus it is safe to say that each part of the symmetric region will remain either in y > 0 or y < 0.

Now we see what happens at the limit points.

- 1. Let $t_0 \in [t/4, 3t]$ be fixed and let $\rho \longrightarrow \infty$. If we do so we see that both horizontal lines stretch out to infinity while the distance between them, $11t_0/4$, remains unchanged. But also, if we look at the slope of the side lines we observe that it tends to zero. This means that the vertical distance compared to the horizontal one is ridiculously small and so we would be looking at a horizontal line, i.e. both initial lines merge into one.
- 2. Let now $\rho = \rho_0$ be fixed and let $t \rightarrow 0$. Clearly the length of the upper and lower lines goes to zero and so does the vertical distance between them. However while this happens the centers of the lines remain still but vertically closer. The key point here is to observe the length of the side lines. Observe that

$$d = \frac{11}{4}\sqrt{t^2 + \rho_0^2} \longrightarrow \frac{11\rho_0}{4}$$

hence these lines do not dissapear but progressively lose inclination till they merge into a unique horizontal line. This means that the region squeezes when t tends to zero until we only see a horizontal line of length $11\rho_0/4$ with start and end points $5\rho_0/4$ and $4\rho_0$ respectively.

Suppose now that the particle moves on a two dimensional space. This could be a plane, say \mathbb{R}^2 . Thus the solution u may be represented as

$$u = u(x, y, t),$$

 $(x, y) \in \mathbb{R}^2$ and $t \in \mathbb{R}$ as usual. In this case, the observability region becomes a surface. For each $s \in [t/4, 3t]$ we see circles instead of lines. The projection of the region is the one on figure 1.1.



Figure 1.1: The projection of the observability region. The axis of the graphic correspond to the spatial variables x and y.

The blue lines correspond to the instant s = t/4. The dashed line is the circle of radius $5\rho/4$ as pointed on figure 1.1 and the lines next to it are the ones defining the region

$$\left| |(x,y)| - \frac{5}{4}\rho \right| < 4\rho\sqrt{t}.$$

Likewise the red lines correspond to the instant s = 3t that define the following region

$$||(x,y)| - 4\rho| < 4\rho\sqrt{t}.$$

It is thus not hard to picture that as s grows we draw annuli of growing radius. This gives place to a conic surface on space for which the shape varies depending on the parameters t and ρ as we studied for the 1 dimensional case.

On the last part of this chapter we are going to analyze the particular case where the particle described by u is periodic in space, meaning that for periodic points of the space the nature of the system does not change. Following a little with the observability results we started mentioning on this section, there are a number of articles regarding the observability problem of periodic solutions, see for instance [46], [44].

Let $\mathbb{T}^2 := \mathbb{R}^2 / A\mathbb{Z} \times B\mathbb{Z}$, $A, B \in \mathbb{R} / \{0\}$ and consider the Schrödinger problem

$$i\partial_t u(z,t) = (-\Delta + V(z))u(z,t), \quad z \in \mathbb{T}^2,$$
(1.43)

where $V \in \mathcal{C}^{\infty}(\mathbb{T}^2)$ is a smooth real valued potential. The following result can be found in [3], a paper by N. Burq and M. Zworski.

Theorem 1.7.1. Let $\Omega \subset \mathbb{T}^2$ be any (non-empty) open set and let T > 0. There exists a constant $K = K(\Omega, T)$, depending only on Ω and T, such that for any solution of (1.43) we have

$$\|u(\cdot,0)\|_{L^{2}(\mathbb{T}^{2})}^{2} \leq K \int_{0}^{T} \|u(\cdot,t)\|_{L^{2}(\Omega)}^{2} dt.$$
(1.44)

Observe that this result involves time independent potentials. Such observability results are still unknown for time dependent potentials.

We see next what happens if we apply our theorem to a periodic solution of our problem. Consider the one dimensional case, so $\mathbb{T} := \mathbb{R}/[0, 2\pi]$. Assume now that we have a periodic in space solution $u \in \mathcal{C}([0, 1]; \mathcal{H}^1(\mathbb{T}))$ of the problem (1.1) and

$$\int_{[-\pi,\pi]} |u_0|^2 dx = c_0^2$$

Choose $\rho = 2\pi$. Then the observability region has the form

$$\left|y \pm 2\pi \left(1 + \frac{s}{t}\right)\right| < 8\pi\sqrt{t}, \quad s \in [t/4, 3t],$$

that by periodicity becomes

$$\left| y \pm 2\pi \frac{s}{t} \right| < 8\pi \sqrt{t}, \quad s \in [t/4, 3t].$$

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Some remarks in the periodic case

If we look carefully now to this region we see that an interesting phenomenon occurs. The solution u goes beyond the point 2π up to three times as s grows from t/4 to 3t for a given value of t, which, we recall, is very small. This happens because the observability region has length larger than 2π . Thus, the solution u may be found several times within the interval $[0, 2\pi]$ and there is no need to observe its behaviour in further points. Here is a sketch of the geometry described by the solution:



The red area corresponds to the original observability region whereas the blue part is the periodic comeback. It is clear that all the information can be gathered if one looks only within the initial ball.

We could re-estate (1.4.1) for a periodic solution as

Proposition 1.7.2. Let $u \in \mathcal{C}([0,1] : \mathcal{H}^1_{loc}(\mathbb{T}))$ be a solution of

$$\begin{cases} \partial_t u = i(\partial_x^2 u + V(x,t)u) \\ u(x,0) = u_0(x), \end{cases}$$

where $V \in L^{\infty}(\mathbb{T} \times [0,1])$ is a complex potential and

$$\parallel V \parallel_{L^{\infty}(\mathbb{T}\times[0,1])} \leq L$$

Let $c_0 > 0$ be such that,

$$\int_{[-\pi,\pi]} |u_0(x)|^2 dx = c_0^2$$

and consider also that

$$\sup_{0 \le t \le 1} \int_{[-\pi,\pi]} |u(x,t)|^2 + |\partial_x u(x,t)|^2 dx = A^2 < +\infty.$$
(1.45)

Then, there exist $t^* = t^*(c_0, L, A)$ and a universal constant c_1 such that if $0 < t < t^*$,

$$\frac{e^{c_1/t}}{t} \int_{t/4}^{3t} \int_{|y \pm 2\pi \frac{s}{t}| < 8\pi\sqrt{t}} |u|^2 + s|\partial_x u|^2 dy ds \ge c_0^2.$$
(1.46)

This result can be seen as some kind of one dimensional observability inequality for periodic solutions of (1.1), as we mentioned earlier. Observe also that the variable t can be small, as estated on Theorem 1.4.1. The drawback of (1.46) is that involves ∇u , and it is a very natural question to know if this term is needed. Also, and because of this dependence on the gradient, it is not clear up to what extent (1.46) implies a controllability result. Nevertheless, observe that our result allows potentials that can depend on time and holds in any dimension.
Chapter 2

The non-elliptic Schrödinger problem

2.1 The hyperbolic equation

Up to this point we worked with Schrödinger's initial value problem on its elliptic version. For this problem we analyzed the quantification of the solution under certain assumptions. This is, we found conditions on the initial data u_0 so that the \mathcal{H}^1 norm of the solution could be controlled from below on certain region of space.

Now we turn to the hyperbolic version of the problem, that is,

$$\begin{cases} \partial_t u = i(\Delta_1 - \Delta_2 + V(x, t))u\\ u(x, 0) = u_0(x), \end{cases}$$
(2.1)

where $x = (x_1, x_2)$ with $x_1 = (x_1^1, x_1^2, ..., x_1^{n_1}) \in \mathbb{R}^{n_1}, x_2 = (x_2^1, x_2^2, ..., x_2^{n_2}) \in \mathbb{R}^{n_2}$ such that $n_1 + n_2 = n$ and the Laplacian operators Δ_1 and Δ_2 are defined as

$$\Delta_1 u = \sum_{i=1}^{n_1} \partial_i^2 u \tag{2.2}$$

$$\Delta_2 u = \sum_{j=n_1+1}^n \partial_j^2 u. \tag{2.3}$$

We also consider the potential depending on the space and time variables. In particular we might consider $V = V(u, \bar{u})$. This kind of allowance on the potential gives rise to non-linear problems for which well-posedness is needed in order to make sense out of the solution. A particular example is to consider the two dimensional equation

$$i\partial_t u + \frac{1}{2}\partial_x^2 u - \frac{1}{2}\partial_y^2 u \pm |u|^2 u = 0, \quad (x,y) \in \mathbb{R}^2,$$
 (2.4)

that appears in nonlinear optics. This problem is locally well-posed in $\mathcal{H}^s(\mathbb{R}^2)$ for any s > 0 and for $L^2(\mathbb{R}^2)$ although global existence remains unclear for the latter. This is due to the fact that the energy defined as

$$E = \|\partial_x u\|_{L^2(\mathbb{R}^2)}^2 - \|\partial_y u\|_{L^2(\mathbb{R}^2)}^2 \mp \|u\|_{L^4(\mathbb{R}^2)}^4,$$

is not positive. However global existence in $\mathcal{H}^{s}(\mathbb{R}^{2})$ for any s > 0 can be obtained via modulation approximation [53].

Our main task in this chapter is to generalize the results from the previous one. We have seen that if the L^2 norm of the initial data is nonzero around the origin and the \mathcal{H}^1 norm of the solution is locally controlled then u and its gradient can be quantified in terms of u_0 . We are now interested in adapting this result to the non-elliptic case of Schrödinger's initial value problem. This task can be done by following the same strategy as before although the result varies a little as we will see.

In order to generalize Theorem 1.4.1, we need to make sure that all the side lemmas we used are consistent to the new equation. We pay special attention to Carleman's lemma for which we need to give a new version for the hyperbolic operator. The proof does not change much but we include it for clearence. The lemma itself is stated in 2.3.1.

The main theorem of this chapter is stated in 2.4.1. There are slight differences with respect to the original result that we will point out along the way but the proof follows the same strategy as the one used in the previous chapter so most of the details will be omitted. The most interesting point is that when the hyperbolic operator acts on the function g of 2.3.1 we have terms depending on the dimensions of the vectors x_1 and x_2 as well as factors of the form $||x_1|^2 - |x_2|^2|$ acting on $|u|^2$ which suggests that the L^2 norm of u might be concentrated near points where $|x_1| = |x_2|$. All the details are gathered in section 4 of the chapter.

We close this chapter with the particular case of a periodic solution of (2.1) in dimension 2. We thus work on the two dimensional thorus $\mathbb{T}^2 := (\mathbb{R}/2\pi\mathbb{Z})^2$ so that problem (2.1) becomes

$$\begin{cases} \partial_t u = i(\partial_x^2 - \partial_y^2 + V(x, y, t))u, \\ u(x, y, 0) = u_0(x, y). \end{cases}$$

We see what happens when a periodic solution of the above problem satisfies conditions of 2.4.1. In 2.5.1 we state the corresponding version of 2.4.1 for a periodic solution.

2.2 The explicit formula for the solution

Before giving the main result of this chapter we need to study the nature of the solution of (2.1). We have previously seen that we can write down an explicit formula for the solution to the free Schrödinger problem

$$\begin{cases} \partial_t u = i\Delta u, \\ u(x,0) = u_0(x), \end{cases}$$
(2.5)

by using the Fourier Transformation. In this case the solution is given by

$$u(x,t) = \frac{e^{i\frac{|x|^2}{4t}}}{(4\pi i t)^{n/2}} \int_{\mathbb{R}^n} e^{-i\frac{x}{2t}y} e^{i\frac{|y|^2}{4t}} u_0(y) \, dy.$$

We would like to do the same for the hyperbolic case. We first try to find an explicit formula of our problem. Again, we use Fourier Transforms to solve the equivalent problem on the frequency space \mathbb{R}^n_{ξ} , say

$$\begin{cases} \partial_t \hat{u} = (\widehat{\Delta_1 - \Delta_2})u = 0\\ \hat{u}(\xi, 0) = \hat{u}_0(\xi). \end{cases}$$

We thus compute the Fourier Transform of each laplacian operator by using the properties we know so that

$$\widehat{\Delta_{1}u}(\xi) = (2\pi)^{-n/2} \int e^{-ix\cdot\xi} \Delta_{1}u(x)dx$$

= $(2\pi)^{-n/2} \int i\xi_{1}e^{-ix\cdot\xi} \nabla_{1}u(x)dx$
= $-|\xi_{1}|^{2}(2\pi)^{-n/2} \int e^{-ix\cdot\xi}u(x)dx$
= $-|\xi_{1}|^{2}\hat{u}(\xi),$

and likewise,

$$\widehat{\Delta_2 u}(\xi) = -|\xi_2|^2 \widehat{u}(\xi).$$

Therefore, combining both calculations and plugging the expressions into the general operator we obtain

$$i(\Delta_1 - \Delta_2)u = -i(|\xi_1|^2 - |\xi_2|^2)\hat{u},$$

which gives

$$\hat{u}(\xi,t) = \hat{u}_0(\xi)e^{-it(|\xi_1|^2 - |\xi_2|^2)},$$

to finally obtain

$$\begin{aligned} u(x,t) &= (2\pi)^{-n/2} \int e^{ix \cdot (\xi_1 + \xi_2) - it(|\xi_1|^2 - |\xi_2|^2)} \hat{u}_0(\xi) d\xi \\ &= (4\pi i t)^{-n/2} e^{i\frac{|x_1|^2 - |x_2|^2}{4t}} \int e^{-it\left(\xi_1 - \frac{x_1}{2t}\right)^2 + it\left(\xi_2 - \frac{x_2}{2t}\right)^2} \hat{u}_0(\xi) d\xi, \\ &= (4\pi i t)^{-n/2} \int e^{i\frac{|x_1 - y_1|^2 - |x_2 - y_2|^2}{2t}} u_0(y) dy, \end{aligned}$$

where $i^{1/2} = e^{i\pi/4}$ for t > 0 and $e^{-i\pi/4}$ for t < 0 as happened for the elliptic case. The last equality is obtained after using a suitable change of variables together with the definition of the Fourier Transform.

2.3 The Carleman estimate

We saw that one of the key points to prove the main theorem of the previous chapter was Carleman's estimate. However, in order to use it we need to see if the lemma works for the hyperbolic equation. This is indeed the case and we present the statement of the lemma together with the proof of it.

Lemma 2.3.1 Carleman estimate. Assume that R > 0 and $\varphi : [0, 1] \longrightarrow \mathbb{R}$ is a smooth function. Then, there exists $\hat{c_n} = c(n, \|\varphi''\|_{\infty}) > 0$ such that the inequality

$$\frac{\sigma^{3/2}}{\hat{c}_n R^2} \| e^{\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} g \|_2 \leq \| e^{\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} (i\partial_t + \Delta_1 - \Delta_2) g \|_2,$$
(2.6)

holds when $\sigma \geq \hat{c_n} R^2$ and $g \in \mathcal{C}_0^{\infty}(\mathbb{R}^{n+1})$ has its support contained in the set

$$\left\{ (x,t) : \left| \frac{x}{R} + \varphi(t)e_1 \right| \ge 1 \right\}.$$

Proof. The proof is very similar to the one of the original Carleman lemma. Let f be a function defined as

$$f(x,t) = e^{\sigma \left| \frac{x}{R} + \varphi e_1 \right|^2} g(x,t),$$

then,

$$\begin{split} e^{\sigma \left|\frac{x}{R} + \varphi e_1\right|^2} (i\partial_t + \Delta_1 - \Delta_2) g(x, t) &= -2i\sigma\varphi' \left(\frac{x_1^1}{R} + \varphi\right) f + i\partial_t f - \frac{2\sigma(n_1 - n_2)}{R^2} \\ &+ \sigma^2 \left[\frac{4}{R^2} \left(\frac{x_1}{R} + \varphi e_1\right)^2 - \frac{4}{R^2} \left(\frac{x_2}{R}\right)^2\right] \\ &- 2\sigma \left[\frac{2}{R} \left(\frac{x_1}{R} + \varphi e_1\right) \nabla_1 f - \frac{2}{R} \frac{x_2}{R} \nabla_2 f\right] \\ &+ (\Delta_1 - \Delta_2) f. \end{split}$$

The Carleman estimate

Now we define

$$S_{\sigma} = i\partial_t + (\Delta_1 - \Delta_2) + \frac{4\sigma}{R^2} \left[\left(\frac{x_1}{R} + \varphi e_1\right)^2 - \left(\frac{x_2}{R}\right)^2 \right],$$

and

$$A_{\sigma} = \frac{i\varphi'}{2} \left(\frac{x_1^1}{R} + \varphi\right) + \frac{n_1 - n_2}{2R^2} + \frac{1}{R} \left[\left(\frac{x_1}{R} + \varphi e_1\right) \nabla_1 - \frac{x_2}{R} \nabla_2 \right],$$

symmetric and anti-symmetric operators respectively. By doing this we can derive the following inequality

$$\begin{aligned} \left\| e^{\sigma \left| \frac{x}{R} + \varphi e_1 \right|^2} (i\partial_t + \Delta_1 - \Delta_2) g \right\|_2^2 &= \langle (S_\sigma - 4\sigma A_\sigma) f, (S_\sigma - 4\sigma A_\sigma) f \rangle \\ &= \left\| S_\sigma f \right\|_2^2 + \left\| A_\sigma f \right\|_2^2 - 4\sigma \langle [S_\sigma, A_\sigma] f, f \rangle \\ &\geq -4\sigma \langle [S_\sigma, A_\sigma] f, f \rangle. \end{aligned}$$

We need to study the commutator. A long calculation shows that

$$[S_{\sigma}, A_{\sigma}] = \frac{2i\varphi'}{R} \partial_1 - \frac{1}{2} \left[\left(\frac{x_1^1}{R} + \varphi \right) \varphi'' + (\varphi')^2 \right] + \frac{2}{R^2} (n_1 \Delta_1 + n_2 \Delta_2) - \frac{8\sigma^2}{R^4} \left| \frac{x_1}{R} + \varphi e_1 \right|^2 - \frac{8|x_2|^2 \sigma^2}{R^6}.$$

Now we plug it into the previous inequality so that

$$\begin{aligned} -4\sigma \langle [S_{\sigma}, A_{\sigma}]f, f \rangle &= -4\sigma \int [S_{\sigma}, A_{\sigma}]f\bar{f}dxdt \\ &= -\frac{8i\sigma}{R} \int \varphi' \partial_1 f\bar{f}dxdt + 2\sigma \int \left[\left(\frac{x_1^1}{R} + \varphi\right)\varphi'' + (\varphi')^2 \right] |f|^2 dxdt \\ &- \frac{8\sigma}{R^2} \int (n_1\Delta_1 + n_2\Delta_2)f\bar{f}dxdt + \frac{8\sigma^3}{R^4} \int \left|\frac{x_1}{R} + \varphi e_1\right|^2 |f|^2 dxdt \\ &+ \frac{32\sigma^3}{R^6} \int |x_2|^2 |f|^2 dxdt. \end{aligned}$$

We now want to find a lower bound for this expression. For this purpose we need to work out some of the integrals and rewrite them so that we can eliminate the ones we do not need. Observe first that,

$$\int (n_1 \Delta_1 + n_2 \Delta_2) f \bar{f} dx dt = -\int (n_1 |\nabla_1 f|^2 + n_2 |\nabla_2 f|^2) dx dt$$

and

$$\begin{aligned} \left|\frac{8\sigma}{R}\int\varphi'\partial_{1}f\bar{f}dxdt\right| &= \left|2\int(\sqrt{2}\sigma^{1/2}\varphi'\bar{f})\left(\frac{2\sqrt{2}}{R}\sigma^{1/2}\partial_{1}f\right)dxdt\right| \\ &\leq 2\sigma\int(\varphi')^{2}|f|^{2}dxdt + \frac{8\sigma}{R^{2}}\int|\nabla_{1}f|^{2}dxdt.\end{aligned}$$

Using these expressions we can give a new lower bound, say

$$\begin{aligned} -4\sigma \langle [S_{\sigma}, A_{\sigma}]f, f \rangle &\geq \frac{8\sigma}{R^2} (n_1 - 1) \int |\nabla_1 f|^2 dx dt + 2\sigma \int \left(\frac{x_1^1}{R} + \varphi\right) \varphi'' |f|^2 dx dt \\ &+ \frac{8\sigma n_2}{R^2} \int |\nabla_2 f|^2 dx dt + \frac{8\sigma^3}{R^4} \int \left|\frac{x_1}{R} + \varphi e_1\right|^2 |f|^2 dx dt \\ &+ \frac{32\sigma^3}{R^6} \int |x_2|^2 |f|^2 dx dt \\ &\geq 2\sigma \int \left(\frac{x_1^1}{R} + \varphi\right) \varphi'' |f|^2 dx dt + \frac{8\sigma^3}{R^4} \int \left|\frac{x_1}{R} + \varphi e_1\right|^2 |f|^2 dx dt.\end{aligned}$$

Observe now that

$$\left|2\sigma \int \left(\frac{x_1^1}{R} + \varphi\right)\varphi''|f|^2 dx dt\right| \le 2\sigma \|\varphi''\|_{\infty} \int \left|\frac{x_1}{R} + \varphi e_1\right| |f|^2 dx dt,$$

which makes the inequality look like

$$-4\sigma\langle [S_{\sigma}, A_{\sigma}]f, f\rangle \geq -2\sigma \|\varphi''\|_{\infty} \int \left|\frac{x_1}{R} + \varphi e_1\right| |f|^2 dx dt + \frac{32\sigma^3}{R^4} \int \left|\frac{x_1}{R} + \varphi e_1\right|^2 |f|^2 dx dt.$$

Considering $|x_1/R + \varphi e_1| \ge 1$ the lemma follows by taking $\sigma \ge \hat{c}_n R^2$ for a constant $\hat{c}_n = c(n, \|\varphi''\|_{\infty})$ as we wanted.

2.4 The main theorem for the hyperbolic case

As we said before we want to follow the same strategy as we did for the elliptic case of the problem. To do so, we also need to apply the Appell's Conformal transformation to the solution. For the solution of the hyperbolic equation this transformation is given by

$$\tilde{u}(x,t) = \left(\frac{\sqrt{\alpha\beta}}{\alpha(1-t)+\beta t}\right)^{n/2} u\left(\frac{\sqrt{\alpha\beta}x}{\alpha(1-t)+\beta t}, \frac{\beta t}{\alpha(1-t)+\beta t}\right) e^{\frac{(\alpha-\beta)(|x_1|^2-|x_2|^2)}{4i(\alpha(1-t)+\beta t)}}$$
(2.7)

For this case we also define $\gamma = \alpha/\beta$ like we did on the previous chapter. Using Carleman's lemma and the Appell Conformal transformation we can give the analogous version of 1.4.1 for the hyperbolic Schrödinger equation as follows

Theorem 2.4.1. Let $u \in \mathcal{C}([0,1] : \mathcal{H}^1_{loc}(\mathbb{R}^n = \mathbb{R}^{n_1} \times \mathbb{R}^{n_2})$ be a solution of

$$\begin{cases} \partial_t u = i(\Delta_1 - \Delta_2 + V(x, t))u\\ u(x, 0) = u_0(x), \end{cases}$$

where $V \in L^{\infty}(\mathbb{R}^n \times [0,1])$ is a complex potential and

$$\parallel V \parallel_{L^{\infty}(\mathbb{R}^n \times [0,1])} \leq L.$$

Let $R_0 > 0$ be such that for some $c_0 > 0$,

$$\int_{B_{R_0}} |u_0|^2 dx = c_0^2,$$

and let also $M \ge 4R_0 + 1$ so that

$$\sup_{0 \le t \le 1} \int_{B_M} |u(x,t)|^2 + |\nabla u(x,t)|^2 dx = A^2 < +\infty.$$
(2.8)

Then, there exist $t^* = t^*(c_0, R_0, A, L)$ and a universal constant c_n that depends just on the dimension such that if $0 < t < t^*$,

$$\frac{e^{c_n\frac{\rho^2}{t}}}{t} \int_{t/4}^{3t} \int_{||y|-\rho-\rho\frac{s}{t}|<4\rho\sqrt{t}} \left| |y_1|^2 - |y_2|^2 \right|^2 |u|^2 + (n_1 - n_2)^2 |u|^2 \qquad (2.9)$$
$$+ |y_1 \cdot \nabla_1 u - y_2 \cdot \nabla_2 u|^2 \ dyds \ge c_0^2,$$

for $R_0 \leq \rho \leq M$.

Remark: Note that if $n_1 = n_2$ then (2.9) looks like

$$\frac{e^{c_n\frac{\rho^2}{t}}}{t}\int_{t/4}^{3t}\int_{||y|-\rho-\rho\frac{s}{t}|<4\rho\sqrt{t}}\left||y_1|^2-|y_2|^2\right|^2|u|^2+|y_1\cdot\nabla_1u-y_2\cdot\nabla_2u|^2\ dyds\geq c_0^2.$$

It might happen that most of the L^2 norm of the solution u is concentrated near the points where $|y_1| = |y_2|$. If that is the case the gradients of u will also take large values but since we are computing the difference between them this quantity may be balanced.

The proof of this result follows the same scheme of the former one. Nevertheless there are slight differences along the proof that we will point out. The strategy is the same, i.e. we define a function g using cut off functions as we did before (1.29). As for these cut off functions, we consider that θ_R is a radial function so that

$$\theta_R(|x|) = \theta_R(r), \quad r = \sqrt{|x_1|^2 + |x_2|^2}.$$

This apreciation is necessary since we are computing derivatives in different directions and the outcome may vary and alter the region of observability, as we will see. Now if we compute the gradient of θ_R for each of the directions x_1 and x_2 we obtain,

$$\nabla_1 \theta_R = \frac{x_1}{|x|} \theta'_R, \qquad \nabla_2 \theta_R = \frac{x_2}{|x|} \theta'_R \tag{2.10}$$

and moreover, we compute also the laplacians,

$$\Delta_1 \theta_R = \theta_R'' \frac{|x_1|^2}{|x|^2} + \theta_R' \frac{n_1 |x|^2 - |x_1|^2}{|x|^3},$$
$$\Delta_2 \theta_R = \theta_R'' \frac{|x_2|^2}{|x|^2} + \theta_R' \frac{n_2 |x|^2 - |x_2|^2}{|x|^3},$$

so that,

$$(\Delta_1 - \Delta_2)\theta_R = \left(|x_1|^2 - |x_2|^2\right) \left(\frac{\theta_R''}{|x|^2} - \frac{\theta_R'}{|x|^3}\right) + (n_1 - n_2)\frac{\theta_R'}{|x|}.$$
 (2.11)

Taking this into account we define the function g exactly as we did for the former proof, say

$$g(x,t) = \theta_R(|x|)\eta\left(\frac{x}{R} + \varphi e_1\right)\tilde{u}(x,t),$$

and apply Carleman's lemma. When we work out the left hand side of the inequality there is no difference with respect to the former proof since we don't have to work with the derivatives of g so we have

$$\| e^{\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} g(x,t) \|_2^2 \ge \frac{e^{8\sigma}}{64} c_0^2, \qquad (2.12)$$

whenever

$$\gamma \ge 2^{14} \left(\frac{A}{c_0}\right)^4,$$

As for the right hand side, when we compute the operator on g we obtain:

$$\begin{aligned} (i\partial_t + \Delta_1 - \Delta_2)g(x,t) &= \tilde{V}g \\ &+ \theta_R (i\varphi'\partial_1\eta\tilde{u} + 2R^{-1}(\nabla_1\eta\nabla_{x_1}\tilde{u} - \nabla_2\eta\nabla_{x_2}\tilde{u}) + R^{-2}(\Delta_1\eta - \Delta_2\eta)\tilde{u}) \\ &+ \eta [(\Delta_1\theta_R - \Delta_2\theta_R)\tilde{u} + 2(\nabla_1\theta_R\nabla_{x_1}\tilde{u} - \nabla_2\theta_R\nabla_{x_2}\tilde{u})] \\ &= E_1 + E_2 + E_3. \end{aligned}$$

Where \tilde{V} satisfies $|\tilde{V}| \leq L\gamma^{-1}$ and the supports of E_2 and E_3 do not change with respect to the original proof so we have, respectively

$$suppE2 \subseteq \left\{ (x,t) \mid 3/2 \le \left| \frac{x}{R} + \varphi(t) \right| \le 2 \quad , \quad t \in [1/4, 3/4] \right\},$$
$$suppE_3 \subseteq \{ R \le |x| \le R+1 \} \times [1/4, 3/4].$$

Using the same argumentation as we did on the proof of 1.4.1 we find the following upper bound to the right hand side of (2.6),

$$\| e^{\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} (i\partial_t + \Delta_1 - \Delta_2)g \|_2^2 \leq L^2 \gamma^{-2} \| e^{\sigma \left| \frac{x}{R} + \varphi(t)e_1 \right|^2} g \|_2^2 + e^{8\sigma} I_1 + e^{72\sigma} I_2,$$

where I_1 and I_2 are the integrals of $|E_2|^2$ and $|E_3|^2$ over the corresponding supports. The first one can be estimated by A as we did before (1.33). The second one however needs a little bit more work since it carries the derivatives of the function θ_R defined in (2.10) and (2.11). We split I_2 so that the calculation is more clear.

$$\begin{split} I_{2}^{1} &= \int_{1/4}^{3/4} \int_{R \leq |x| \leq R+1} \left| (\Delta_{1} - \Delta_{2}) \theta_{R} \tilde{u} \right|^{2} dx dt \\ &= \int_{t} \int_{x} \left| \left(|x_{1}|^{2} - |x_{2}|^{2} \right) \left(\frac{\theta_{R}''}{|x|^{2}} - \frac{\theta_{R}'}{|x|^{3}} \right) + (n_{1} - n_{2}) \frac{\theta_{R}'}{|x|} \right|^{2} |\tilde{u}|^{2} dx dt \\ &\leq \int_{t} \int_{x} \left| R^{-3} (|x_{1}|^{2} - |x_{2}|^{2}) ((R+1)\theta_{R}'' - \theta_{R}') + R^{-1} (n_{1} - n_{2}) \right|^{2} |\tilde{u}|^{2} dx dt \\ &\leq c R^{-2} \int_{t} \int_{x} \left| |x_{1}|^{2} - |x_{2}|^{2} \right|^{2} |\tilde{u}|^{2} + (n_{1} - n_{2})^{2} |\tilde{u}|^{2} dx dt. \end{split}$$

Now we plug in the definition of \tilde{u} (2.7) together with the change of variables

$$y = \alpha(t)x, \quad s = s(t),$$

where $\alpha(t)$ and s(t) were defined in (1.15) and (1.16) respectively. We also use the estimates (1.23) and (1.26) so that all together gives the following upper bound

$$\begin{split} I_{2}^{1} &\leq cR^{-2} \int_{t} \int_{x} \left| |x_{1}|^{2} - |x_{2}|^{2} \right|^{2} \alpha(t)^{n} |u(\alpha(t)x, s(t))|^{2} + (n_{1} - n_{2})^{2} \alpha(t)^{n} |u(\alpha(t)x, s(t))|^{2} dx dt \\ &\leq c\gamma R^{-2} \int_{s(1/4)}^{s(3/4)} \int_{\alpha R \leq |y| \leq \alpha(R+1)} \alpha^{-4} \left| |x_{1}|^{2} - |x_{2}|^{2} \right|^{2} |u(y, s)|^{2} + (n_{1} - n_{2})^{2} |u(y, s)|^{2} dy ds \\ &\leq cR_{0}^{2} \gamma^{2} \int_{s(1/4)}^{s(3/4)} \int_{\alpha R \leq |y| \leq \alpha(R+1)} \left| |x_{1}|^{2} - |x_{2}|^{2} \right|^{2} |u(y, s)|^{2} + (n_{1} - n_{2})^{2} |u(y, s)|^{2} dy ds. \end{split}$$

For the last step we also used the definition of R, say $R = R_0 \sqrt{\gamma}$. Before resuming with the estimation of I_2 we compute the gradient of our solution \tilde{u} for each vector x_1 and x_2 . The expressions we obtain are

$$\nabla_{x_1}\tilde{u} = \alpha(t)^{n/2} e^{-\frac{i}{4}\beta(t)|x|^2} \left(\alpha(t)\nabla_1\tilde{u} - \frac{i}{2}\beta(t)x_1\tilde{u}\right),$$
$$\nabla_{x_2}\tilde{u} = \alpha(t)^{n/2} e^{-\frac{i}{4}\beta(t)|x|^2} \left(\alpha(t)\nabla_1\tilde{u} - \frac{i}{2}\beta(t)x_2\tilde{u}\right),$$

where $\beta(t)$ was defined in (1.17). Now we are ready to work out the second part

of integral I_2 ,

$$\begin{split} I_{2}^{2} &\leq 4 \int_{1/4}^{3/4} \int_{R \leq |x| \leq R+1} |\nabla_{1}\theta_{R} \nabla_{x_{1}}\tilde{u} - \nabla_{2}\theta_{R} \nabla_{x_{2}}\tilde{u}|^{2} dx dt \\ &\leq 4R^{-2} \int_{t} \int_{x} |x_{1} \cdot \nabla_{x_{1}}\tilde{u} - x_{2} \cdot \nabla_{x_{2}}\tilde{u}|^{2} dx dt \\ &= 4R^{-2} \int_{t} \int_{x} \alpha(t)^{n} |x_{1}(\alpha(t)\nabla_{1}u(\alpha(t)x, s(t)) - \frac{i}{2}\beta(t)x_{1}u(\alpha(t)x, s(t))) \\ &- x_{2}(\alpha(t)\nabla_{2}u(\alpha(t)x, s(t)) - \frac{i}{2}\beta(t)x_{2}u(\alpha(t)x, s(t)))|^{2} dx dt \\ &= 4R^{-2} \int_{t} \int_{x} \alpha(t)^{n} |\alpha(x_{1} \cdot \nabla_{1}u - x_{2} \cdot \nabla_{2}u) - \frac{i}{2}\beta(|x_{1}|^{2} - |x_{2}|^{2})u|^{2} dx dt \\ &\leq 4\gamma R^{-2} \int_{s} \int_{y} |(y_{1} \cdot \nabla_{1}u(y, s) - y_{2} \cdot \nabla_{2}u(y, s)) - \frac{i}{2}\beta\alpha^{-2}(|y_{1}|^{2} - |y_{2}|^{2})u(y, s)|^{2} dy ds \\ &\leq 4R_{0}^{2}\gamma^{2} \int_{s} \int_{y} ||y_{1}|^{2} - |y_{2}|^{2}|^{2} |u|^{2} + |y_{1} \cdot \nabla_{1}u - y_{2} \cdot \nabla_{2}u|^{2} dy ds. \end{split}$$

Now if we put all together and use (1.23) and (1.27) we have

$$\begin{split} I_2 &\leq cR_0^2 \gamma^2 \int_{s \sim \gamma^{-1}} \int_{||y| - R_0 - R_0 s \gamma| < \frac{4R_0}{\sqrt{\gamma}}} \left| |x_1|^2 - |x_2|^2 \right|^2 |u(y,s)|^2 + (n_1 - n_2)^2 |u(y,s)|^2 \\ &+ |y_1 \cdot \nabla_1 u - y_2 \cdot \nabla_2 u|^2 \, dy ds. \end{split}$$

The rest of the proof is the same as the one of 1.4.1.

2.5 The periodic case

As we did on the previous chapter we want to see what happens if we take periodic solutions of (2.1). We are going to consider the two dimensional problem so we are going to be working on the thorus $\mathbb{T}^2 := \mathbb{R}^2/(2\pi\mathbb{Z})^2$. In this context we have the Cauchy problem written as

$$\begin{cases} \partial_t u = i(\partial_x^2 - \partial_y^2 + V(x, y, t))u = 0\\ u(x, y, 0) = u_0(x, y), \end{cases}$$

where we consider the solution u to be periodic in space and the initial data satisfies the following condition

$$\int_{[-\pi,\pi]\times[-\pi,\pi]} |u_0(x,y)|^2 dx dy = c_0^2, \qquad (2.13)$$

for some $c_0 > 0$. Consider also that

$$\sup_{0 \le t \le 1} \int_{[-\pi,\pi] \times [-\pi,\pi]} |u(x,y,t)|^2 + |\nabla u(x,y,t)|^2 dx dy = A^2 < +\infty.$$

The periodic case

Then we can apply the theorem. Considering the solution u is 2π -periodic we have that 2.9 is evaluated on the following region

$$\left| |(x,y)| + 2\pi \frac{s}{t} \right| < 8\pi \sqrt{t}$$

It is clear that we are representing annuli of different radius that get bigger as s grows. Recall also that the contribution of u is not seen on the lines y = x and y = -x. The projection onto the plane would look like this:



The blue circle corresponds to the smallest time s = t/4. As s grows the annuli gets wider generating a cone-shaped form in space. The red circle corresponds to the time s = 3t. The green square corresponds to $[-\pi, \pi] \times [-\pi, \pi]$. We see that the blue circle lies within the square but at some point it exceeds these limits and goes beyond the area. When this happens the information carried by u comes back to the origin by periodicity. Thus we see several cone shaped geometries at different levels corresponding to each value of s.

As for the yellow and purple lines, these correspond to the points where the L^2 norm of the solution u may be concentrated. As it happened for the non periodic

case, it should be analyzed what the behaviour of the solution is when approaching these points.

We can thus rephrase theorem 2.4.1 for the periodic solution as

Proposition 2.5.1. Let $u \in \mathcal{C}([0,1] : \mathcal{H}^1_{loc}(\mathbb{T}^2))$ be a solution of

$$\begin{cases} \partial_t u = i(\partial_x^2 - \partial_y^2 + V(x, y, t))u\\ u(x, y, 0) = u_0(x, y), \end{cases}$$

where $V \in L^{\infty}(\mathbb{T}^2 \times [0,1])$ is a complex potential and

$$\parallel V \parallel_{L^{\infty}(\mathbb{T}^2 \times [0,1])} \leq L.$$

Let $c_0 > 0$ be such that,

$$\int_{[-\pi,\pi]\times[-\pi,\pi]} |u_0(x,y)|^2 dx dy = c_0^2$$

and consider also that

$$\sup_{0 \le t \le 1} \int_{[-\pi,\pi] \times [-\pi,\pi]} |u(x,y,t)|^2 + |\nabla u(x,y,t)|^2 dx dy = A^2 < +\infty.$$

Then, there exist $t^* = t^*(c_0, A, L)$ and a universal constant c such that if $0 < t < t^*$,

$$\frac{e^{\frac{c}{t}}}{t} \int_{t/4}^{3t} \int_{||(x,y)| \pm 2\pi \frac{s}{t}| < 8\pi\sqrt{t}} |x^2 - y^2|^2 |u|^2 + |x\partial_x u - y\partial_y u|^2 \, dxdyds \ge c_0^2.$$

Chapter 3

The Σ_{δ} space and the Virial Theorem

3.1 Introduction

We saw on previous chapters that conditions on the initial data u_0 of Schrödinger's initial value problem granted information about the solution at times t > 0. In particular we have seen how on the perturbative case conditions of this kind together with size conditions on the potential allowed us to control the \mathcal{H}^1 norm of the solution u of the problem from below. Now we turn to the free particle case, say

$$\begin{cases} \partial_t u = \frac{i}{2} \Delta u \\ u(x,0) = u_0(x), \end{cases}$$
(3.1)

where the constant 1/2 on the right hand side is written by convenience. We have seen that for a solution u of the problem the quantity $|u(x,t)|^2$ defines a probability density such that

$$\int_{\mathbb{R}^n} |u(x,t)|^2 dx = 1,$$

for all time t that a priori we consider positive. This means, as we already know, that the probability to find the particle somewhere in space is absolute, as it should. However we would like to quantify this probability for specific regions of space.

As we mentioned we want to find conditions on the initial data that tell us something about the solution u. The motivation of this chapter comes from Theorem 3.1 of [4] where one of the hypothesis of the theorem 1 is

$$\int_{t \sim 1/2} \int_{|x| < 1} |u(x, t)|^2 dx \ge 1.$$
(3.2)

We thus want to find conditions on the initial data so that (3.2) holds. However, we are going to give (3.2) with the lower bound 1/2 instead of 1. This fact does not change the outcome of Theorem 3.1 in [4]. In fact it only affects to the constant c of (1.9).

In section 3.2 we introduce the space Σ_{δ} . This space is the collection of functions satisfying the following condition

$$\int_{\mathbb{R}^n} |x|^{2\delta} |f(x)|^2 dx + |D^{\delta} f(x)|^2 dx < +\infty,$$
(3.3)

for $\delta > 0$ and D^{δ} is the fractional derivative defined via Fourier as

$$D^{\delta}f(x) = \int_{\mathbb{R}^n} e^{ix\cdot\xi} |\xi|^{\delta} \hat{f}(\xi) d\xi.$$

We will later see how restrictive the conditions on δ are and that if the initial data u_0 satisfies (3.3) then so does its evolution in time. This fact will be used to prove (3.2).

The key point in this analysis will be the study of the function

$$h_{\delta}(t) = \int_{\mathbb{R}^n} |x|^{2\delta} |u(x,t)|^2 dx,$$

as we shall see. For this analysis we make use of Pitt's lemma 3.3.1 and the results in [28] by J. Nahas and G. Ponce.

The following section introduces the Virial Theorem. The goal of this result is the same as before, this is, we look for conditions on the initial data that allows us control the L^2 norm of the solution u from below. The main object of study in this section is the function

$$h(t) = \int_{\mathbb{R}^n} \phi(x) |u(x,t)|^2 dx,$$

for a suitable function ϕ of which we talk later. We will analyze the characteristics of this function and see how for specific ϕ we can deliver information about the behaviour of the quantum system defined by u, just like we have done previously.

We finish this chapter by giving a counterexample concerning (3.2). To build this counterexample we make use of the Galilean transformation

$$u_{\lambda}(x,t) = e^{-\frac{i}{2}t|\lambda|^2 + i\lambda \cdot x} u(x - \lambda t, t),$$

for $\lambda \in \mathbb{R}$.

¹Note that in Theorem 3.1 of [4] the condition that u is normalized is not given

3.2 The Σ_{δ} space

As mentioned, the main goal is to find conditions on the initial data u_0 to find lower bounds to the L^2 norm of the solution u on a space-time cylinder. To sort this out we somehow need to control the evolution in time of the system.

First of all we define the following quantities upon the initial data,

$$a_{\delta}^{2} := \int_{\mathbb{R}^{n}} |x|^{2\delta} |u_{0}(x)|^{2} dx, \qquad (3.4)$$

and

$$b_{\delta}^{2} := \int_{\mathbb{R}^{n}} |\xi|^{2\delta} |\hat{u}_{0}(\xi)|^{2} d\xi, \qquad (3.5)$$

where we consider $\delta > 0$ for now and see later what conditions should this parameter satisfy. We also ask for

$$a_{\delta} + b_{\delta} < +\infty. \tag{3.6}$$

The goal is thus to see that these quantities are finite as time goes by, this is, that a solution u of (3.1) generated from u_0 satisfies

$$\int_{\mathbb{R}^n} |x|^{2\delta} |u(x,t)|^2 + |D^{\delta}u(x,t)|^2 dx < +\infty.$$
(3.7)

Observe that δ may be a real number and so we are dealing with fractional derivatives. This is no inconvenience at all. In fact, using Plancherel's theorem and the properties of the Fourier Transform we see that

$$\int_{\mathbb{R}^n} |D^{\delta} u(x,t)|^2 dx = \int_{\mathbb{R}^n} |\xi|^{2\delta} |\hat{u}(\xi,t)|^2 d\xi,$$

which also suggests that if a solution u satisfies (3.7) so does its Fourier Transformation.

We define the Σ_{δ} space as the collection of functions satisfying (3.6) and the norm of this space be given as

$$||f||_{\Sigma_{\delta}}^{2} = \int_{\mathbb{R}^{n}} |x|^{2\delta} |f(x)|^{2} + |D^{\delta}f(x)|^{2} dx$$
(3.8)

The question now is the following: if we take the initial data $u_0 \in \Sigma_{\delta}$, will its evolution in time also belong in this space?

We thus assume that (3.6) is satisfied. We have seen that if a function belongs in the Σ_{δ} space so does its Fourier Transformation. Using this fact and the fact that \hat{u} has the same size as \hat{u}_0 we see that

$$\int_{\mathbb{R}^n} |D^{\delta} u(x,t)|^2 dx = \int_{\mathbb{R}^n} |\xi|^{2\delta} |\hat{u}(\xi,t)|^2 d\xi$$
$$= \int_{\mathbb{R}^n} |\xi|^{2\delta} |\hat{u}_0(\xi)|^2 d\xi < +\infty.$$

The Σ_{δ} space and the Virial Theorem

Our job now is to verify that

$$h_{\delta}(t) = \int_{\mathbb{R}^n} |x|^{2\delta} |u(x,t)|^2 dx, \qquad (3.9)$$

is finite.

3.3 The analysis of the function h_{δ}

In this section we deal with the boundedness of the function h_{δ} defined above (3.9). We have not discussed what should δ be like other than it should be positive. We see what conditions are needed for our purposes. We give the proof of the boundedness of the function h_{δ} in dimension 1 and considering that the time parameter is t = 1. Once this is done, we use a dilation argument to generalize the result to times t > 0. Finally we generalize it to multiple dimensions.

We rewrite the function h_{δ} by using the properties of the Fourier Transform.

$$h_{\delta}(1) = \int_{\mathbb{R}} x^{2\delta} |u(x,1)|^2 dx = \int_{\mathbb{R}} |x^{\delta} u(x,1)|^2 dx$$
$$= \int_{\mathbb{R}} |\widehat{(\cdot)^{\delta} u}(\xi,1)|^2 d\xi$$
$$= \int_{\mathbb{R}} |D^{\delta} \hat{u}(\xi,1)|^2 d\xi$$
$$= \int_{\mathbb{R}} |D^{\delta} (e^{-i\xi^2} \hat{u}_0(\xi))|^2 d\xi$$
$$= \int_{\mathbb{R}} |D^{\delta} (\hat{f}\hat{g})|^2 d\xi,$$

where $\hat{f}(\xi) = e^{-\frac{i}{2}\xi^2}$ and $\hat{g}(\xi) = \hat{u}_0$. We want to see that h_{δ} is bounded. This is done in an article by J. Nahas and G. Ponce, see [28]. One of the key arguments is the use of the following inequality,

$$\|D^{\delta}(\hat{f}\hat{g}) - \hat{f}(D^{\delta}\hat{g}) - (D^{\delta}\hat{f})\hat{g}\|_{2} \le c\|\hat{f}\|_{\infty}\|D^{\delta}\hat{g}\|_{2},$$
(3.10)

that was proved in [17] by C. Kenig, G. Ponce and L. Vega.

The right hand side of (3.10) is finite by assumption. It remains to see whether the term $(D^{\delta}\hat{f})\hat{g}$ is bounded in L^2 . We write

$$\begin{split} \| (D^{\delta} \hat{f}) \hat{g} \|_{2}^{2} &= \int | (D^{\delta} \hat{f}) \hat{g} |^{2} d\xi \\ &= \int_{|\xi| < 1} | (D^{\delta} \hat{f}) \hat{g} |^{2} d\xi + \int_{|\xi| > 1} | (D^{\delta} \hat{f}) \hat{g} |^{2} d\xi \\ &= I + II. \end{split}$$

The analysis of the function h_{δ}

The choice of where we cut the space is not random as we will see later. This appreciation is necessary since the function $D^{\delta}\hat{f}$ grows with each derivative so we need some control over this. When the variable ξ is small we should not have any trouble as we will see shortly. However the case $|\xi| > 1$ is a little more delicate and we need to work it out a little bit more. We thus check both I and II and see that we can bound the L^2 norm of the mentioned product. We begin by analyzing what happens with I:

$$\begin{split} I &= \int_{|\xi|<1} |(D^{\delta}\hat{f})\hat{g}|^2 d\xi \leq \int_{\mathbb{R}} \eta(\xi) |(D^{\delta}\hat{f})\hat{g}|^2 d\xi \\ &\leq \|\eta D^{\delta}\hat{f}\|_{\infty}^2 \|\hat{g}\|_2^2, \end{split}$$

where η is a smooth cut-off function vanishing outside $\{|\xi| < 2\}$. We thus need to check that $u_0 \in L^2$ and that $D^{\delta}(e^{-\frac{i}{2}\xi^2}) \in L^{\infty}$. To answer the first question we use Pitt's inequality:

Lemma 3.3.1 Pitt's inequality. For $f \in \mathcal{S}(\mathbb{R}^n)$ and $0 \leq \alpha < n$, then

$$\int_{\mathbb{R}^n} |x|^{-\alpha} |f(x)|^2 dx \le C_\alpha \int_{\mathbb{R}^n} |y|^\alpha |\hat{f}(y)|^2 dy,$$

where

$$C_{\alpha} = \pi^{\alpha} \left[\Gamma \left(\frac{n-\alpha}{4} \right) / \Gamma \left(\frac{n+\alpha}{4} \right) \right]$$

Thus by using this inequality we can write

$$\int |x|^{-2\alpha} |u_0|^2 dx \lesssim \int |\xi|^{2\alpha} |\hat{u_0}|^2 d\xi = h_{\delta}(+\infty),$$

and so,

$$||u_0||_2^2 = \int |u_0|^2 dx \le \left(\int x^{-2\alpha} |u_0|^2 dx\right) \left(\int x^{2\alpha} |u_0|^2 dx\right) < +\infty$$

Now we want to see that $D^{\delta} \hat{f}$ is bounded. Using the definition of the fractional derivative, together with the fact that the Fourier Transform of the Gaussian is the function itself up to some constants, we have

$$D^{\delta} \hat{f} = D^{\delta} (e^{-\frac{i}{2}\xi^2}) = \int e^{\frac{i}{2}x^2} e^{ix\xi} |x|^{\delta} dx$$
$$= \int_{|x|<1} e^{\frac{i}{2}x^2} e^{ix\xi} |x|^{\delta} dx + \int_{|x|>1} e^{\frac{i}{2}x^2} e^{ix\xi} |x|^{\delta} dx.$$

Here again, as we did with the variable ξ we need to separate the cases close to the origin and the one around infinity. The first integral on the right hand side

is clearly bounded if we take absolute values so we focus on the second term. By completing the square we can rewrite it as

$$\begin{split} \int_{|x|>1} e^{\frac{i}{2}x^2} e^{ix\xi} |x|^{\delta} dx &= e^{-i\frac{\xi^2}{2}} \int_{|x|>1} e^{\frac{i}{2}(x+\xi)^2} |x|^{\delta} dx \\ &= e^{-i\frac{\xi^2}{2}} \left[\int_{\substack{|x+\xi|<1\\|x|>1}} e^{\frac{i}{2}(x+\xi)^2} |x|^{\delta} dx + \int_{\substack{|x+\xi|>1\\|x|>1}} e^{\frac{i}{2}(x+\xi)^2} |x|^{\delta} dx \right] \end{split}$$

Considering as we are that $|\xi| < 1$ the first integral is bounded if we take absolute values. As for the second one, we need to use integration by parts. Before that, we rewrite it as:

$$\int_{\substack{|x+\xi|>1\\|x|>1}} e^{\frac{i}{2}(x+\xi)^2} |x|^{\delta} dx = \int_{\substack{|x+\xi|>1\\|x|>1}} \frac{|x|^{\delta}}{i |x+\xi|} \frac{d}{dx} \left(e^{\frac{i}{2}(x+\xi)^2} \right) dx.$$

When we integrate by parts we see that the integrand can be bounded by

$$\frac{|x|^{\delta-1}}{|x+\xi|},$$

which is integrable only if $\delta < 1$. Observe also that the fact that |x| > 1 was necessary here. Gathering all the above estimations, we see that

$$I \le c \|g\|_2.$$

We now study the contribution of II. The argumentation is very similar to the first case so we are not going to go through all the details. For the first step though, we do a little trick in order to control the derivatives of \hat{f} .

$$II = \int_{|\xi|>1} |(D^{\delta}\hat{f})\hat{g}|^{2}d\xi = \int_{|\xi|>1} |(|\xi|^{-\delta}D^{\delta}\hat{f})(|\xi|^{\delta}\hat{g})|^{2}d\xi$$
$$\leq ||D^{\delta}\hat{f}||_{\infty}^{2} ||\cdot|^{\delta}\hat{g}||_{2}^{2}$$

The term on the right of the product is bounded by hypothesis so we only need to check the boundedness of the term on the left, which is a fractional derivative. We try to rewrite it differently and see if we can find a proper bound:

$$\begin{split} |\xi|^{-\delta} D^{\delta} \hat{f} &= |\xi|^{-\delta} D^{\delta} (e^{-\frac{i}{2}\xi^{2}}) = |\xi|^{-\delta} \int e^{\frac{i}{2}x^{2}} e^{ix\xi} |x|^{\delta} dx \\ &= |\xi|^{-\delta} \left[\int_{|x|<1} e^{\frac{i}{2}x^{2}} e^{ix\xi} |x|^{\delta} dx + \int_{|x|>1} e^{\frac{i}{2}x^{2}} e^{ix\xi} |x|^{\delta} dx \right] \end{split}$$

which is the same situation as before. The first integral gives no problem and we only need to focus on the second one. We can write it exactly like we did in the previous case, say:

$$\begin{split} \int_{|x|>1} e^{\frac{i}{2}x^2} e^{ix\xi} |x|^{\delta} dx &= e^{-i\frac{\xi^2}{2}} \int_{|x|>1} e^{\frac{i}{2}(x+\xi)^2} |x|^{\delta} dx \\ &= e^{-i\frac{\xi^2}{2}} \left[\int_{\substack{|x+\xi|<1\\|x|>1}} e^{\frac{i}{2}(x+\xi)^2} |x|^{\delta} dx + \int_{\substack{|x+\xi|>1\\|x|>1}} e^{\frac{i}{2}(x+\xi)^2} |x|^{\delta} dx \right] \end{split}$$

we analyze first the integral over $|x + \xi| < 1$. Observe first that

$$|x| = |x + \xi - \xi| < |x + \xi| + |\xi| < 1 + |\xi| < 2|\xi|.$$

Using this we can estimate the integral by

$$\int_{|x+\xi|<1} e^{\frac{i}{2}(x+\xi)^2} |x|^{\delta} dx < |\xi|^{\delta} \int_{|x+\xi|<1} e^{\frac{i}{2}(x+\xi)^2} dx$$

which is clearly bounded if we take absolute values and remember that there is a $|\xi|^{-\delta}$ factor multiplying outside. We now look at the integral over $|x + \xi| > 1$. Again, as we did in the case of I, we use integration by parts on the following integral,

$$\int_{\substack{|x+\xi|>1\\|x|>1}} e^{\frac{i}{2}(x+\xi)^2} |x|^{\delta} dx = \int_{\substack{|x+\xi|>1\\|x|>1}} \frac{|x|^{\delta}}{i|x+\xi|} \frac{d}{dx} \left(e^{\frac{i}{2}(x+\xi)^2} \right) dx.$$

Here again when we integrate by parts we see that the integrand is bounded by a factor that is integrable only if $\delta < 1$ exactly as before. We thus see that the integral II is bounded by $c \|D^{\delta}\hat{g}\|_2$.

All in all we have seen that

$$\|(D^{\delta}\hat{f})\hat{g}\|_{2} \le c(\|\hat{g}\|_{2} + \|D^{\delta}\hat{g}\|_{2}).$$
(3.11)

Now we have all the needed estimations, we go back to the definition of the function h_{δ} and write

$$\begin{split} h_{\delta}(1) &= \int_{\mathbb{R}} |D^{\delta}(\hat{f}\hat{g})|^{2} d\xi = \int_{\mathbb{R}} |D^{\delta}(\hat{f}\hat{g}) - (D^{\delta}\hat{f})\hat{g} + (D^{\delta}\hat{f})\hat{g}|^{2} d\xi \\ &\leq c \left(\int_{\mathbb{R}} |D^{\delta}(\hat{f}\hat{g}) - (D^{\delta}\hat{f})\hat{g}|^{2} d\xi + \int_{\mathbb{R}} |(D^{\delta}\hat{f})\hat{g}|^{2} d\xi \right) \\ &\leq c \left(\int_{\mathbb{R}} |\hat{f}(D^{\delta}\hat{g})|^{2} d\xi + \int_{\mathbb{R}} |(D^{\delta}\hat{f})\hat{g}|^{2} d\xi \right) \\ &\leq c \left[\|\hat{f}\|_{\infty}^{2} \|D^{\delta}\hat{g}\|_{2}^{2} + c_{t} (\|\hat{g}\|_{2}^{2} + \|D^{\delta}\hat{g}\|_{2}^{2}) \right] \\ &\leq c \left(\|\hat{g}\|_{2}^{2} + \|D^{\delta}\hat{g}\|_{2}^{2} \right). \end{split}$$

Once the boundedness of h_{δ} is proved for time t = 1 we can use an argument of dilations to prove it for all t. We define

$$u_{\lambda}(x,t) = \lambda^{n/2} u(\lambda x, \lambda^2 t),$$

or rather,

$$u(x,t) = \lambda^{-n/2} u_{\lambda} \left(\frac{x}{\lambda}, \frac{t}{\lambda^2} \right),$$

for any $\lambda > 0$. We thus see that

$$h_{\delta}(t) = \lambda^{-n} \int_{\mathbb{R}} x^{2\delta} \left| u_{\lambda} \left(\frac{x}{\lambda}, \frac{t}{\lambda^2} \right) \right|^2 dx = \lambda^{2\delta} \int_{\mathbb{R}} x^{2\delta} \left| u_{\lambda} \left(x, \frac{t}{\lambda^2} \right) \right|^2 dx.$$

Now we choose $\lambda^2 = t$ so that $u_{\lambda}\left(x, \frac{t}{\lambda^2}\right) = u_{\lambda}(x, 1)$ and the fact that for t = 1 we already know the bound is true so that

$$h_{\delta}(t) = t^{\delta} \int_{\mathbb{R}} x^{2\delta} |u_{\lambda}(x,1)|^{2} dx$$

$$\leq ct^{\delta} \left(\int_{\mathbb{R}} \lambda^{n} x^{2\delta} |u_{0}(\lambda x)|^{2} x^{2\delta} dx + \lambda^{-n} \int_{\mathbb{R}} \xi^{2\delta} \left| \hat{u}_{0} \left(\frac{\xi}{\lambda} \right) \right|^{2} d\xi \right)$$

$$= ct^{\delta} \left(t^{-\delta} \int_{\mathbb{R}} x^{2\delta} |u_{0}(x)|^{2} dx + t^{\delta} \int_{\mathbb{R}} \xi^{2\delta} |\hat{u}_{0}(\xi)|^{2} d\xi \right).$$

From where we have the following upper bound,

$$h_{\delta}(t) \le c(1+t^{2\delta}) \|u_0\|_{\Sigma_{\delta}}$$
 (3.12)

To finish with the analysis of the boundednes of h_{δ} we see that it also works for dimensions greater than 1. Assume again that $u_0 \in \Sigma_{\delta}$ and t = 1. First we make the following observation

$$\int_{\mathbb{R}^n} |x|^{2\delta} |u(x,1)|^2 dx \le \max_{1 \le j \le n} \int_{\mathbb{R}^n} |x_j|^2 |u(x,1)|^2 dx.$$

For simplicity we take j = 1. We write

$$u(x,1) = \int_{\mathbb{R}^n} e^{ix \cdot \xi} \hat{u}(\xi,1) d\xi = \int_{\mathbb{R}^n} e^{ix \cdot \xi - \frac{i}{2}|\xi|^2} \hat{u}_0(\xi) d\xi$$
$$= \int_{\mathbb{R}^{n-1}} e^{i\bar{x} \cdot \bar{\xi} - \frac{i}{2}|\bar{\xi}|^2} \left(\int_{\mathbb{R}} e^{ix_1\xi_1 - \frac{i}{2}\xi_1} \hat{u}_0(\xi_1,\bar{\xi}) d\xi \right) d\bar{\xi}$$

Observe that the term in parenthesis is $u(x_1, \bar{\xi}, 1) = u_{x_1}(\bar{\xi}, 1)$ hence using Plancherel's identity we have that

$$\int_{\mathbb{R}^{n-1}} |u_{x_1}(\bar{x},1)|^2 d\bar{x} = \int_{\mathbb{R}^{n-1}} \left| \int_{\mathbb{R}} e^{ix_1\xi_1 - \frac{i}{2}\xi_1} \hat{u_0}(\xi_1,\bar{\xi}) d\xi \right|^2 d\bar{\xi}.$$

Using this identity we can now estimate

$$\begin{split} \int_{\mathbb{R}^n} |x_1|^{2\delta} |u(x,1)|^2 d\bar{x} dx_1 &= \int_{\mathbb{R}^{n-1}} \left(\int_{\mathbb{R}} |x_1|^{2\delta} |u_{x_1}(\bar{\xi},1)|^2 dx_1 \right) d\bar{\xi} \\ &\leq c(1+t^{2\delta}) \int_{\mathbb{R}^{n-1}} \int_{\mathbb{R}} |x_1|^{2\delta} |u_0(x_1,\bar{\xi})|^2 + |D_1^{\delta} u_0(x_1,\bar{\xi})|^2 dx_1 d\bar{\xi} \\ &\leq c(1+t^{2\delta}) \|u_0\|_{\Sigma_{\delta}}^2. \end{split}$$

which is bounded by assumption. Observe that we have used the fact that the norm of Σ_{δ} is bounded in dimension 1.

All results above lead to the following theorem:

Proposition 3.3.2. Let u be a solution of (3.1) with initial data $u_0 \in \Sigma_{\delta}$. Then $u(\cdot, t) \in \Sigma_{\delta}$ for every t > 0 and $0 < \delta < 1$. Moreover,

$$\|u(\cdot,t)\|_{\Sigma_{\delta}} \le c_{\delta}(1+t^{2\delta})\|u_0\|_{\Sigma_{\delta}}.$$

Observe that we consider δ to be strictly smaller than 1 and that we named the constant c_{δ} in order to differenciate it from the constant that we are going to use for the case $\delta = 1$. It is worth mentioning that in this case such constant is not explicit. The case $\delta = 1$ will be treated later via the Virial Theorem.

Now that we proved h_{δ} is bounded we are ready to find lower bounds to the L^2 norm of the solution as in (3.2). Assume that for $u \in \Sigma_{\delta}$,

$$\int_{\mathbb{R}^n} |u(x,t)|^2 dx = 1$$

Let now $c_0 > 0$ to be defined later. We see that

$$\begin{split} \int_{|x|>c_0} |u(x,t)|^2 dx &= \int_{|x|>c_0} \frac{|x|^{2\delta}}{|x|^{2\delta}} |u(x,t)|^2 dx \\ &\leq c_0^{-2\delta} \int_{|x|>c_0} |x|^{2\delta} |u(x,t)|^2 dx \\ &\leq c_0^{-2\delta} h_{\delta}(t) \\ &\leq c_0^{-2\delta} c_{\delta}(1+t^{2\delta}) \|u_0\|_{\Sigma_{\delta}}. \end{split}$$

Now we compute,

$$\begin{split} 1 &= \int_{\mathbb{R}^n} |u(x,t)|^2 dx = \int_{|x| < c_0} |u(x,t)|^2 dx + \int_{|x| > c_0} |u(x,t)|^2 dx \\ &\implies \int_{|x| < c_0} |u(x,t)|^2 dx = 1 - \int_{|x| > c_0} |u(x,t)|^2 dx \\ &\implies \int_{|x| < c_0} |u(x,t)|^2 dx \ge 1 - c_0^{-2\delta} c_\delta (1+t^{2\delta}) \|u_0\|_{\Sigma_\delta} \end{split}$$

We want to see that the mass within the ball B_{c_0} is greater than 1/2. This being so we impose the following condition on our parameter,

$$c_0^{-2\delta} c_\delta(1+t^{2\delta}) \|u_0\|_{\Sigma_\delta} \le \frac{1}{2} \Longrightarrow c_0^{2\delta} \ge 2c_\delta(1+t^{2\delta}) \|u_0\|_{\Sigma_\delta}.$$

We have thus proved the following result

Corollary 3.3.3. Let $u \in \mathcal{C}([0, +\infty); \Sigma_{\delta})$ be the solution to Schrödinger's initial value problem

$$\begin{cases} \partial_t u = \frac{i}{2} \Delta u \\ u(x,0) = u_0(x) \end{cases}$$

where u_0 satisfies (3.4) and (3.5) for $0 < \delta < 1$. Then for $c_0 = (2c_{\delta}(1 + t^{2\delta}) \|u_0\|_{\Sigma_{\delta}})^{1/2\delta}$ the following holds

$$\int_{|x|
(3.13)$$

Remark: Observe that c_0 depends on time and can be large. However for $t \leq 1$ the parameter c_0 is uniform in time.

We would like to extend this result to non-linear problems. In Chapter 1 we already saw how allowing complex potentials depending on the space time variables together with a nice well-posedness theory of the non-linear problem can bring about complementary results. This being so assume we have the following problem,

$$\begin{cases} i\partial_t u + \Delta u = \mu |u|^{a-1} u, \quad t \in \mathbb{R}, \quad x \in \mathbb{R}^n, \quad \mu = \pm 1, \quad a > 1\\ u(x,0) = u_0(x). \end{cases}$$
(3.14)

The natural question here is what happens if we choose $u_0 \in \Sigma_{\delta}$. Is the solution to (3.14) going to belong in Σ_{δ} as well?

To answer this question we refer to [28] an article by J. Nahas and G. Ponce in which they present various results regarding the dynamical behaviour of the solution u locally. We are going to mention some of them in order to give a more general overview. The main result is the following,

Theorem 3.3.4. Let $s_c = n/2 - 2/(a-1)$

1. If $s > s_c$, $s \ge 0$, with $[s] \le a - 1$ if a is not an odd integer, then for each $u_0 \in H^s(\mathbb{R}^n)$ there exist $T = T(||u_0||_{s,2}) > 0$ and a unique solution u = u(x,t) of (3.14) with

 $u \in C\left(\left[-T, T\right] : H^{s}\left(\mathbb{R}^{n}\right)\right) \cap L^{q}\left(\left[-T, T\right] : L^{p}_{s}\left(\mathbb{R}^{n}\right)\right) = Z^{s}_{T}$

Moreover, the map data \rightarrow solution is locally continuous from $H^s(\mathbb{R}^n)$ into Z_T^s

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2. If $s = s_c$ and $s \ge 0$, then part (I) holds with $T = T(u_0) > 0$

where for $1 and <math>s \in \mathbb{R}$

$$L_s^p(\mathbb{R}^n) \equiv (1-\Delta)^{-s/2} L^p(\mathbb{R}^n), \quad \|\cdot\|_{s,p} \equiv \|(1-\Delta)^s \cdot\|_p,$$

and the indices (q, p) above are given by the Strichartz estimate

$$\left(\int_{-\infty}^{\infty} \left\| e^{it\Delta} u_0 \right\|_p^q dt \right)^{1/q} \le c \left\| u_0 \right\|_2,$$

where

$$\frac{n}{2} = \frac{2}{q} + \frac{n}{p}, \quad 2 \le p \le \infty, \text{ if } n = 1, \quad 2 \le p < 2n/(n-2), \text{ if } n \ge 2.$$

We thus see how the regularity of the solution u is continuously preserved in time. However we need the extra condition that controls the decay in space so that we make sure we still have solutions of the space Σ_{δ} . This is also proved in [28] by P. Nahas and G. Ponce in the following theorem.

Theorem 3.3.5. In addition to the hypothesis in Theorem 3.3.4 assume that $u_0 \in L^2(|x|^{2\delta}dx)$ $\delta > 0$ with $[m] \leq a-1$ if a is not an odd integer. If $s \geq \delta$ then

$$u \in C\left([-T,T]: H^{s} \cap L^{2}\left(|x|^{2\delta}dx\right)\right) \cap L^{q}\left([-T,T]: L_{s}^{p} \cap L^{p}\left(|x|^{2\delta}dx\right) = Z_{T}^{s,\delta},$$
(3.15)

with p and q as in Theorem 3.3.4.

We thus see that if the initial data u_0 lives in the space $\mathcal{H}^s \cap L^2(|x|^{2\delta}dx)$ then the solution u is preserved in time and lives in a space contained in Σ_{δ} . Therefore the function h_{δ} will be bounded for solutions u of the non-linear problem and times $t \in [0, T]$, as we wanted to see.

Following the same proof as in 3.3.3 we have the following theorem

Theorem 3.3.6. If all conditions in theorem (3.3.5) are satisfied then the solution u of (3.14) belongs in Σ_{δ} . Moreover, $h_{\delta}(t)$ is bounded for $t \in [0, T]$ and there exists $c_0 = c_0(T)$ such that

$$\int_{|x| < c_0} |u(x,t)|^2 dx \ge \frac{1}{2}.$$

Now we want to use this information to give an alternative version of Theorem 3.1 in [4]. However this theorem requires the potential to be bounded. Problem (3.14) gives the potential in terms of the solution u so we need it to belong in L^{∞} . This can be done by the Sobolev embedding theorem if we take the number of derivatives s to be greater than n/2. We can thus give the following result,

Corollary 3.3.7. Let $u_0 \in \mathcal{H}^s(\mathbb{R}^n) \cap L^2(|x|^{\delta})$ with s > n/2 and $0 < \delta < 1$. Then the solution u of (3.14) satisfies (3.15) and there exist $R_0 = R_0(n, ||u||_{\mathcal{H}^1}, ||u||_{\infty})$ and c = c(n) such that for any $R \ge R_0$

$$\left(\int_{-T}^{T} \int_{R-1 < |x| < R} \left(|u|^2 + |\nabla_x u|^2 \right)(x, t) dx dt \right)^{1/2} \ge c e^{-cR^2}$$

3.4 The Virial Theorem

In the previous section we saw how the L^2 norm for functions $u \in \Sigma_{\delta}$ was bounded from below on a space-time cylinder when $\delta < 1$. In this section we want to reach the same conclusion but using a different approach. In this case we are going to make use of the Virial Theorem. The main tool of this theorem is the following function

$$h(t) = \int_{\mathbb{R}^n} \phi(x) |u(x,t)|^2 dx,$$
(3.16)

where ϕ is generally a function with polynomial growth so that all the computations are carried away smoothly and u is the solution of Schrödinger's initial value problem where no potential V is involved. Notice that the function h_{δ} defined previously is a particular case of h. We will address this fact later.

The first part of this section is devoted to some calculations performed upon h. More specifically we will compute the derivatives of the function that, for especific well chosen functions ϕ will allow us to say something about the solution u.

The natural space to work in when we are dealing with quantum systems are Hilbert Spaces, because they are linear vector spaces on which we can define operators representing physical magnitudes. This being so, we represent the function h as an inner product as follows:

$$h(t) = \langle \phi u, u \rangle, \tag{3.17}$$

and we compute the first and second derivatives using the properties of the inner product,

$$\begin{split} h'(t) &= \partial_t \langle \phi u, u \rangle = \langle \phi u_t, t \rangle + \langle \phi u, u_t \rangle \\ &= \langle \phi \frac{i}{2} \Delta u, u \rangle + \langle \phi u, \frac{i}{2} \Delta u \rangle \\ &= \frac{i}{2} \langle \phi \Delta u, u \rangle - \frac{i}{2} \langle \phi u, \Delta u \rangle \\ &= \frac{i}{2} [\langle \phi \Delta u, u \rangle - \langle \Delta (\phi u), u \rangle \\ &= \frac{i}{2} \langle (\phi \Delta - \Delta \phi) u, u \rangle = -\frac{i}{2} \langle Au, u \rangle, \end{split}$$

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where A is the anti symmetric operator given by the commutator $[\Delta, \phi]$. Observe that when the laplacian acts on the product ϕu we have that,

$$\Delta(\phi u) = (\nabla \cdot \nabla)(\phi u) = \nabla(\nabla \phi + \phi \nabla)u = \Delta \phi u + 2\nabla \phi \nabla u + \phi \Delta u, \qquad (3.18)$$

and thus $Au = (\Delta \phi + 2\nabla \phi \nabla)u$. For convenience we also write the explicit formulation of h', say

$$h'(t) = -\frac{i}{2} \langle Au, u \rangle = -\frac{i}{2} \int_{\mathbb{R}^n} (\Delta \phi + 2\nabla \phi \cdot \nabla) u \bar{u} dx$$
$$= -\frac{i}{2} \int_{\mathbb{R}^n} \Delta \phi |u|^2 + 2\nabla \phi \cdot \nabla u \bar{u} dx.$$

We only need to worry about the real part of this expression. If we do so we get

$$h'(t) = Im \int_{\mathbb{R}^n} \nabla \phi \cdot \nabla u \bar{u} dx.$$

As for the second derivative, we have

$$\begin{split} h''(t) &= -\frac{i}{2} \partial_t \langle Au, u \rangle = -\frac{i}{2} [\langle Au_t, u \rangle + \langle Au, u_t \rangle] \\ &= -\frac{i}{2} [\langle A(\frac{i}{2} \Delta u, u \rangle + \langle Au, \frac{i}{2} \Delta u \rangle] \\ &= \frac{1}{4} [\langle A \Delta u, u \rangle - \langle Au, \Delta u \rangle] \\ &= -\frac{1}{4} [\langle \Delta u, Au \rangle + \langle Au, \Delta u \rangle] \\ &= -\frac{1}{2} Re \langle \Delta u, Au \rangle = \frac{1}{2} Re \langle \nabla u, \nabla (Au) \rangle \\ &= \frac{1}{2} Re \langle \nabla u, \nabla (Au) \rangle + \frac{1}{2} Re \langle \nabla u, A \nabla u \rangle - \frac{1}{2} Re \langle \nabla u, A \nabla u \rangle \\ &= \frac{1}{2} Re \langle \nabla u, (\nabla A - A \nabla) u \rangle + \frac{1}{2} Re \langle \nabla u, A \nabla u \rangle, \end{split}$$

where the last term vanishes as A is an anti-symmetric operator. All in all we have that

$$h''(t) = \frac{1}{2} Re \langle \nabla u, (\nabla A - A \nabla) u \rangle.$$

Next we want to make a closer study of the commutator $[\nabla, A]$. We see that,

$$\begin{aligned} (\nabla A - A\nabla)u &= \nabla Au - A\nabla u \\ &= \nabla (\Delta \phi + 2\nabla \phi \nabla)u - A\nabla u \\ &= \nabla (\Delta \phi)u + \Delta \phi \nabla u + 2D^2 \phi \nabla + 2\nabla \phi D^2 u - A\nabla u \\ &= \nabla (\Delta \phi)u + \Delta \phi \nabla u + 2D^2 \phi \nabla + 2\nabla \phi D^2 u - (\Delta \phi + 2\nabla \phi \nabla) \nabla u \\ &= \nabla (\Delta \phi)u + \Delta \phi \overline{\forall u} + 2D^2 \phi \nabla + 2\nabla \phi D^2 \overline{u} - \Delta \phi \overline{\forall u} - 2\nabla \phi D^2 \overline{u} \\ &= \nabla (\Delta \phi)u + 2D^2 \phi \nabla u \end{aligned}$$

and plug it in the previous equation so that

$$\begin{split} h''(t) &= \frac{1}{2} Re \langle \nabla u, (\nabla A - A \nabla) u \rangle = \frac{1}{2} Re \langle \nabla u, \nabla (\Delta \phi) u + 2D^2 \phi \nabla u \rangle \\ &= \frac{1}{2} Re \langle \nabla u, \nabla (\Delta \phi) u \rangle + \langle \nabla u, D^2 \phi \nabla u \rangle \\ &= -\frac{1}{4} \langle u, \Delta^2 \phi u \rangle + \langle \nabla u, D^2 \phi \nabla u \rangle. \end{split}$$

The following lemma is thus proved:

Lemma 3.4.1. Let u be a solution to the Schrödinger initial value problem in the Schwarz class and ϕ a function with polynomial growth. If h is defined as in (3.17), then

$$h''(t) = -\frac{1}{4} \int_{\mathbb{R}^n} \Delta^2 \phi(x) |u(x,t)|^2 dx + \int_{\mathbb{R}^n} \nabla u D^2 \phi \nabla \bar{u} dx.$$
(3.19)

Remark: The operator D^2 refers to the Hessian matrix. In this case it is applied to our function $\phi = \phi(x)$,

$$D^{2}\phi = \begin{pmatrix} \frac{\partial^{2}\phi}{\partial x_{1}^{2}} & \cdots & \frac{\partial^{2}\phi}{\partial x_{1}\partial x_{n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial^{2}\phi}{\partial x_{n}\partial x_{1}} & \cdots & \frac{\partial^{2}\phi}{\partial x_{n}^{2}} \end{pmatrix}$$

Regarding 3.4.1 it is convenient to calculate the bilaplacian operator of ϕ together with the Hessian matrix we just mentioned. For convenience we are going to assume that our function ϕ is radial, say $\phi = \phi(r)$ where r = |x|. Having this on mind, we see that:

$$\partial_j \phi = \frac{x_j}{|x|} \phi', \qquad j = 1, ..., n$$

$$\partial_j^2 \phi = \frac{|x|^2 - x_j^2}{|x|^3} \phi' + \frac{x_j^2}{|x|^2} \phi'', \quad \partial_i \partial_j \phi = -\frac{x_i x_j}{|x|^3} \phi' + \frac{x_i x_j}{|x|^2} \phi'', \quad i, j = 1, ..., n$$

These are the entries of the Hessian matrix, say

$$D^{2}\phi(|x|) = \begin{pmatrix} \frac{|x|^{2} - x_{1}^{2}}{|x|^{3}}\phi' + \frac{x_{1}^{2}}{|x|^{2}}\phi'' & \dots & -\frac{x_{1}x_{n}}{|x|^{3}}\phi' + \frac{x_{1}x_{n}}{|x|^{2}}\phi'' \\ \vdots & \ddots & \vdots \\ -\frac{x_{n}x_{1}}{|x|^{3}}\phi' + \frac{x_{n}x_{1}}{|x|^{2}}\phi'' & \dots & \frac{|x|^{2} - x_{n}^{2}}{|x|^{3}}\phi' + \frac{x_{n}^{2}}{|x|^{2}}\phi'' \end{pmatrix}$$

As for the bilaplacian operator, some calculations give the following expression:

$$\Delta^2 \phi(|x|) = -\frac{(n-1)(n-3)}{|x|^3} \phi' + \frac{(n-1)(n-3)}{|x|^2} \phi'' + \frac{2(n-1)}{|x|} \phi''' + \phi^{iv}.$$

The case $\phi(|x|) = |x|^2$

We see from this expression that depending on the dimension of the problem we might have difficulties defining the sign of the bilaplacian. Lemma 3.4.1 tells us that we are interested in taking the bilaplacian negative so that we can find a lower positive bound to h''. We will later see how we should consider working on the euclidean space of dimension greater than 3 so that everything works out fine.

Once we have defined the first and second derivatives of h for a general function ϕ it is time to see some particular cases.

3.5 The case $\phi(|x|) = |x|^2$

We see that the function h defines the action of the solution of (3.1) with a suitable radial function ϕ . On this section we analyze the case where this function is $|x|^2$. Thus the function h is written as

$$h(t) = \int_{\mathbb{R}^n} |xu(x,t)|^2 dx, \quad t \in \mathbb{R}.$$
(3.20)

We have talked about how $|u|^2$ defines a density function on a probability space and that how this fact is connected to the certainty to find the particle somewhere in space. Since we are talking about probabilities, recall that the symmetric operator S = x defines the position of the quantum system and thus (3.20) carries information about the dispersion of the quantum system.

Another observation is that this function is a particular case of h_{δ} , more precisely, the case $\delta = 1$. We have already talked about it, nevertheless, the case $\delta = 1$ has some interesting properties that we would like to point out. As we did in the first section and also because they play a very important role on the whole computation, we define the following numbers:

$$a^{2} := \int_{\mathbb{R}^{n}} |xu_{0}(x)|^{2} dx < +\infty, \qquad (3.21)$$

and,

$$b^{2} := \int_{\mathbb{R}^{n}} |\nabla u_{0}(x)|^{2} dx < +\infty, \qquad (3.22)$$

which give us information about the position and the momentum of the initial data u_0 . Recall that these magnitudes satisfy the following,

$$1 = \int_{\mathbb{R}^n} |u_0(x)|^2 dx = \frac{2}{n} \operatorname{Re} \int_{\mathbb{R}^n} x \cdot \nabla u \bar{u} dx$$

$$\leq \frac{2}{n} \left(\int_{\mathbb{R}^n} |x u_0(x)|^2 dx \right)^{1/2} \left(\int_{\mathbb{R}^n} |\nabla u_0(x)|^2 dx \right)^{1/2}$$

$$= \frac{2}{n} ab.$$

Another observation is that we can assume by dilations that a = b. In fact for $\lambda > 0$ we define

$$u_{\lambda}(x,t) = \lambda^{-n/2} u(\lambda^{-1}x, \lambda^{-2}t).$$
(3.23)

It can easily be seen that u_{λ} is also a solution of (3.1). Using the new solutions we just described we define,

$$a_{\lambda}^{2} := \int |xu_{0}^{\lambda}(x)|^{2} dx = \int \lambda^{-n} |xu_{0}(\lambda^{-1}x)|^{2} dx$$
$$= \lambda^{2} \int |xu_{0}(x)|^{2} = (\lambda a)^{2},$$
$$b_{\lambda}^{2} := \int |\nabla u_{0}^{\lambda}(x)|^{2} dx = \int \lambda^{-n-2} |\nabla u_{0}(\lambda^{-1}x)|^{2} dx$$
$$= \lambda^{-2} \int |\nabla u_{0}|^{2} dx = (b/\lambda)^{2}.$$

Now we choose λ such that $a_{\lambda} = b_{\lambda}$. If we do so we have the following relation

$$(\lambda a)^2 = (b/\lambda)^2 \Longrightarrow \lambda^2 = b/a.$$

The first part of this section will focus on the analysis of the function h itself considering the results obtained on the previous section. Then we will use this information to conclude (3.2).

Since ϕ is a radial function,

$$\phi'(r) = 2r, \qquad \phi''(r) = 2,$$

which by easy computation gives us:

$$D^2\phi = 2I_n, \qquad \Delta^2\phi = 0,$$

where I_n is the identity matrix of dimension n. Now if we use lemma 3.4.1 we obtain

$$h''(t) = 2 \int_{\mathbb{R}^n} |\nabla u(x,t)|^2 dx.$$
 (3.24)

This immediatly tells us that h is a convex function. Recall now that if u is a solution of (3.1) then the quantity $||u(\cdot, t)||_2$ is constant so

$$\frac{d}{dt}\int_{\mathbb{R}^n}|u(x,t)|^2dx=0.$$

Since ∇u is also a solution of (3.1) we see that

$$\frac{d}{dt}\int_{\mathbb{R}^n} |\nabla u(x,t)|^2 dx = 0.$$

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The case $\phi(|x|) = |x|^2$

This means that h'' is constant and thus

$$h''(t) = h''(0).$$

Using this information we get

$$h(t) = h(0) + h'(0)t + \frac{1}{2}h''(0)t^2.$$
(3.25)

From the definitions of the parameters a and b we see that

$$h(0) = \int |xu_0(x)|^2 dx = a^2,$$

$$h''(0) = 2 \int |\nabla u_0(x)|^2 dx = b^2,$$

and hence,

$$h(t) = a^2 + th'(0) + t^2b^2.$$

So we are able to write the function h using nothing but the information we have for the initial time. It is clear that h defines a convex parabola. Considering that h has to be positive for all t by definition, we are able to represent it as a graph G(t, h(t)) as shown on the following image:



where t_0 is the minimum that can be explicitly calculated:

$$t_0 = -\frac{h'(0)^2}{2b^2}.$$

Next we make a few **remarks**:

1. By translation in time we may assume that the minimum of the function h is attained at time t = 0, i.e., h'(0) = 0. In this case, the function h can be written as

$$h(t) = a^2 + b^2 t^2. aga{3.26}$$

2. Using the uncertainty principle on the parameters a and b, say $1 \leq 2ab$, we have that

$$h(t) = a^{2} + b^{2}t^{2} \ge \frac{1}{4b^{2}} + b^{2}t^{2}, \qquad (3.27)$$

the last expression being also a parabola. It is straight forward to see that both parabolas coindice everywhere if 2ab = 1, this is, when the uncertainty principle becomes an equality. We also know that the function that satisfies this minimizing condition is the Gaussian, i.e.

$$u_0(x) = e^{-|x|^2/2}$$

Later we will see another approach to this matter where we find an upper bound of h and see how one of the functions minimizing the problem is precisely the Gaussian as well.

Assume now that for each $t \in \mathbb{R}$ the probability to find the particle is 1, this is, the solution exists for every t on the given interval, say

$$1=\int_{\mathbb{R}^n}|u(x,t)|^2dx$$

Let now $c_0 > 0$ to be defined later and compute

$$\begin{split} \int_{|x|>c_0} |u(x,t)|^2 dx dt &= \int_{|x|>c_0} \frac{|x|^2}{|x|^2} |u(x,t)|^2 dx \\ &\leq \frac{1}{c_0^2} \int_{|x|>c_0} |xu|^2 dx \\ &\leq \frac{1}{c_0^2} h(t) \\ &= \frac{a^2 + b^2 t^2}{c_0^2}. \end{split}$$

We want this quantity to be less than 1/2, this is, the mass concentrated outside the ball B_{c_0} to be less than the one concentrated inside. This imposition suggests that c_0 has to satisfy the following:

$$c_0 \ge \sqrt{2}\sqrt{a^2 + b^2 t^2}.$$

Having this in mind we see that

$$\int_{|x| < c_0} |u(x,t)|^2 dx \ge \frac{1}{2},$$

for $t \in \mathbb{R}$. We have proved the following result:

Proposition 3.5.1. Let $u \in C(\mathbb{R}; H^1(\mathbb{R}^n))$ be the solution of (3.1) where u_0 satisfies (3.21) and (3.22). Then for $c_0 = \sqrt{2}\sqrt{a^2 + b^2t^2}$ the following holds

$$\int_{|x| \le c_0} |u(x,t)|^2 dx \ge \frac{1}{2},\tag{3.28}$$

for every $t \in \mathbb{R}$.

Remark: The parameter c_0 grows linearly with t. If $t \leq 1$ then we can take $c_0 \geq \sqrt{2}\sqrt{a^2 + b^2}$.

To sum up, we see that for $\delta \in (0, 1]$ condition (3.28) is achieved. The difference between the cases $\delta < 1$ and $\delta = 1$ is that the parameter c_0 is explicit in the latter, which is not the case for the former and depends on c_{delta} defined in 3.3.2.

3.6 The Galilean transformation and a counterexample

In this section we give a counterexample concerning (3.2). We look yet again at Schrödinger's initial value problem (3.1). We want to generate a new family of solutions depending on a parameter. Let thus $\lambda \in \mathbb{R}^n$ be a given vector and define

$$v_0(x) = e^{i\lambda \cdot x} u_0(x) \tag{3.29}$$

as the initial data of the problem

$$\begin{cases} \partial_t v = \frac{i}{2} \Delta v \\ v(x,0) = v_0(x). \end{cases}$$
(3.30)

We know that the solution to this problem verifies the following identity:

$$\hat{v}(\xi, t) = \hat{v}_0(\xi) e^{-\frac{i}{2}t|\xi|^2}$$

where,

$$\hat{v}_0(\xi) = \int e^{-ix\cdot\xi} v_0(x) dx = \int e^{-ix\cdot\xi} e^{i\lambda\cdot x} u_0(x) dx$$
$$= \int e^{-ix(\xi-\lambda)} u_0(x) dx = \hat{u}_0(\xi-\lambda).$$

We use these calculations to compute the solution v,

$$\begin{split} v(x,t) &= \int e^{ix\cdot\xi} \hat{v}(\xi,t) d\xi = \int e^{ix\cdot\xi} \hat{v}_0(\xi) e^{-\frac{i}{2}t|\xi|^2} d\xi \\ &= \int e^{ix\cdot\xi} e^{-\frac{i}{2}t|\xi|^2} \hat{u}_0(\xi-\lambda) d\xi \\ &= \int e^{ix\cdot(\mu+\lambda)} e^{-\frac{i}{2}t|\mu+\lambda|^2} \hat{u}_0(\mu) d\mu \\ &= e^{i\lambda\cdot x} \int e^{ix\cdot\mu} e^{-\frac{i}{2}t|\mu|^2} e^{-\frac{i}{2}t|\lambda|^2} e^{-it\lambda\cdot\mu} \hat{u}_0(\mu) d\mu \\ &= e^{-\frac{i}{2}t|\lambda|^2+i\lambda\cdot x} \int e^{i\mu\cdot(x-\lambda t)} e^{-\frac{i}{2}t|\mu|^2} \hat{u}_0(\mu) d\mu \\ &= e^{-\frac{i}{2}t|\lambda|^2+i\lambda\cdot x} u(x-\lambda t,t). \end{split}$$

We have thus proved the following lemma:

Lemma 3.6.1. Let u be a solution to the homogeneous Schrödinger problem with initial data u_0 and let $\lambda \in \mathbb{R}^n$ be a vector. Then the function $u_{\lambda}(x,t) = e^{-\frac{i}{2}t|\lambda|^2 + i\lambda \cdot x}u(x - \lambda t, t)$ is also a solution of the original problem.

We use now this result to construct an example of a solution u for which the L^2 norm tends to 0. Let

$$u_0(x) = e^{-|x|^2/2}$$

the Gaussian for which we also know that its Fourier Transform is

$$\hat{u}_0(\xi) = e^{-\frac{|\xi|^2}{2}}.$$

Now we can give the explicit definition of the Fourier Transform of the solution u, say

$$\hat{u}(\xi,t) = e^{-\frac{|\xi|^2}{2}(1+it)},$$

which leads to

$$u(x,t) = \frac{1}{(1+it)^{n/2}} e^{-\frac{|x|^2}{2(1+it)}},$$
(3.31)

for t > 0. We apply now the Galilean transformation of 3.6.1 to (3.31). Let thus $\lambda \in \mathbb{R}^n$ be such that $|\lambda| >> 1$, so that

$$u_{\lambda}(x,t) = e^{-\frac{i}{2}t|\lambda|^2 + i\lambda \cdot x}u(x-\lambda t,t)$$
$$= \frac{1}{(1+it)^{n/2}}e^{-\frac{i}{2}t|\lambda|^2 + i\lambda \cdot x}e^{-\frac{|x-\lambda t|^2}{2(1+it)}}$$

We also see that for t = 0,

$$u_{\lambda}(x,0) = e^{i\lambda \cdot x} u_0(x) = e^{i\lambda \cdot x} e^{-|x|^2/2}.$$
(3.32)

Observe that if we compute the L^2 of the initial data inside the ball of radius 1 we have,

$$\int_{|x|<1} |u_{\lambda}(x,0)|^2 dx = \int_{|x|<1} e^{-|x|^2} dx \ge 2e^{-1} = c_0,$$

We see what happens if we compute the L^2 norm of its evolution in time:

$$\int_{1/2}^{1} \int_{|x|<1} |u_{\lambda}(x,t)|^2 dx dt = \int_{1/2}^{1} \int_{|x|<1} |u(x-\lambda t,t)|^2 dx dt$$
$$\sim \frac{1}{2} Vol(B_1) |u(0-\lambda t,t)|^2$$
$$\sim e^{-|\lambda|^2/2} := A^2,$$

which decays exponentially in λ and thus we cannot control it uniformly from below as it was expected. What happens?

Observe that

$$\nabla u_{\lambda}(x,0) = e^{i\lambda \cdot x} (i\lambda u_0(x) + \nabla u_0(x))$$

 $\mathrm{so},$

$$|\nabla u_{\lambda}(x,0)| \gtrsim |\lambda| \longrightarrow \infty.$$

As it was expected, one of the assumptions of 3.5.1 is not satisfied by (3.32). More concretely, the quantity b is not finite hence the L^2 norm of the solution cannot be uniformly bounded from below.

The Σ_{δ} space and the Virial Theorem

Chapter 4 Dynamical Uncertainty Principles

4.1 Introduction

In the previous chapter we analyzed the function h_{δ} for $0 < \delta \leq 1$ where the case $\delta = 1$ was treated differently for its particular characteristics. We have seen that this function is bounded for finite time intervals and therefore we could control the L^2 norm of the solution u on a space-time cylinder of space. These upper bounds give rise to dynamical principles for the function h_{δ} . In this chapter we analyze this matter.

The upper bounds for the function h_{δ} were given in terms of the Σ_{δ} norm of the initial data u_0 and the time parameter. However we want to rewrite these bounds in terms of the solution u. To do so we write it as $u = \rho e^{i\theta}$ where both ρ and θ are real valued functions depending on space and time variables.

This definition of the solution u will allow us to find upper bounds to h_{δ} in terms of the functions ρ and θ that will describe a dynamical uncertainty principle. Once this is done our job will be to find the solutions u that minimize the problem.

We separate this task for the cases $\delta = 1$ first and $\delta < 1$ after. The former has the advantage that it can be treated explicitly since h_1 describes a parabola as we have already seen. In particular we have seen that due to Heisenberg's Uncertainty Principle we have

$$h(t) = a^2 + b^2 t^2 \ge \frac{1}{4b^2} + b^2 t^2,$$

where equality is only attained when 1 = 2ab. Further, we know that this condition implies that equality only holds when the initial data u_0 is the Gaussian function.

As we said all the computations for the case $\delta = 1$ can be done explicitly. The extra advantage, as we will see, is that the case $\delta < 1$ inherits most of the characteristics of the previous problem. This being so, we will see that the problem of finding the minimizers of the Uncertainty Principle is reduced to solving a system of partial differential equations.

4.2 A minimizing problem

In this section we are going to study a dynamical uncertainty principle related to the dispersion of the quantum system described by u. We saw in previous sections that the function h defined in (3.20) could be explicitly written in terms of the position and momentum of the initial data so that

$$h(t) = \int_{\mathbb{R}^n} |x|^2 |u(x,t)|^2 dx = a^2 + b^2 t^2, \tag{4.1}$$

if h'(0) = 0.

Where we could also assume a = b by a dilation argument. Next we write the solution u as

$$u(x,t) = \rho(x,t)e^{i\theta(x,t)}, \qquad (4.2)$$

where ρ and θ are both real functions. We want to study the behaviour of these functions to find upper bounds for h. As we move forward in this analysis we will see different properties that functions ρ and θ must satisfy. By plugging (4.2) into the integral definition of h we get

$$h(t) = \int_{\mathbb{R}^n} |x|^2 |\rho(x,t)|^2 dx.$$
(4.3)

We see that h is independent of the argument function θ as it should be. Recall that the first derivative of h is given by

$$h'(t) = 2Im \int_{\mathbb{R}^n} x \cdot \nabla u \bar{u} dx, \qquad (4.4)$$

and by taking the absolute value and using Cauchy-Schwarz's inequality we have

$$|h'(t)| = \left| 2Im \int_{\mathbb{R}^n} x \cdot \nabla u \bar{u} dx \right|$$

$$\leq 2 \left(\int_{\mathbb{R}^n} |xu(x,t)|^2 dx \right)^{1/2} \left(\int_{\mathbb{R}^n} |\nabla u(x,t)|^2 dx \right)^{1/2}$$

We want to do the same thing but in terms of the functions ρ and θ to see what this inequality looks like. If we compute the derivative of u from (4.2) we see that

$$\nabla u(x,t) = (\nabla \rho + i\rho \nabla \theta)e^{i\theta}, \qquad (4.5)$$
and we plug it into (4.4) so that

$$\begin{aligned} |h'(t)| &= \left| 2Im \int_{\mathbb{R}^n} x \cdot \nabla u \bar{u} dx \right| \\ &= \left| 2Im \int_{\mathbb{R}^n} x (\nabla \rho + i\rho \nabla \theta) e^{i\theta} \rho e^{-i\theta} dx \right| \\ &= \left| 2 \int_{\mathbb{R}^n} x \cdot \nabla \theta \rho^2 dx \right|. \end{aligned}$$

And we use Cauchy-Schwarz's inequality again on this expression to obtain

$$|h'(t)| \le 2\left(\int_{\mathbb{R}^n} |x\rho|^2 dx\right)^{1/2} \left(\int_{\mathbb{R}^n} |\rho\nabla\theta|^2 dx\right)^{1/2}.$$
(4.6)

We have thus redefined the uncertainty principle in terms of ρ and θ . We go a step further and see that by using (4.3) we have

$$\frac{|h'(t)|}{2h(t)^{1/2}} \le \left(\int_{\mathbb{R}^n} |\rho \nabla \theta|^2 dx\right)^{1/2}.$$
(4.7)

Considering as we are that the parabola described by h has its minimum at t = 0 we can write (4.7) as

$$\frac{h'(t)}{2h(t)^{1/2}} \le \left(\int_{\mathbb{R}^n} |\rho \nabla \theta|^2 dx\right)^{1/2},$$
(4.8)

if we consider t > 0. Integrating both sides of the equation in time we have,

$$h^{1/2}(t) \le a + \int_0^t \left(\int_{\mathbb{R}^n} |\rho \nabla \theta|^2 dx \right)^{1/2} ds.$$
 (4.9)

Something similar can be done for t < 0. Our goal is to minimize this problem, or rather, find ρ and θ so that the inequality (4.9) becomes an equality. In order to find these functions, we need to establish certain conditions. The first one is found by looking at (4.6) because we know that equality holds when

$$\nabla \theta(x,t) = \lambda(t)x, \tag{4.10}$$

or,

$$\partial_r \theta = r\lambda(t). \tag{4.11}$$

for a function $\lambda(t)$ that we later define. We also see by integrating (4.10) that the function θ is given by

$$\theta(x,t) = \frac{1}{2}\lambda(t)|x|^2 + \varphi(t), \qquad (4.12)$$

for some function φ only depending on time that we will define later. It is clear from (4.12) that the function θ is radial.

We go back to (4.7) and see that by using (4.10) we have

$$\begin{aligned} \frac{|h'(t)|}{2h(t)^{1/2}} &= \left(\int_{\mathbb{R}^n} |\rho \nabla \theta|^2 dx\right)^{1/2} \\ &= \lambda(t) \left(\int_{\mathbb{R}^n} |x\rho|^2 dx\right)^{1/2} \\ &= \lambda(t)h(t)^{1/2}. \end{aligned}$$

From where we conclude that

$$\lambda(t) = \frac{|h'(t)|}{2h(t)}.$$

Now since h is an explicit function we can calculate λ with no problem, say

$$\lambda(t) = \frac{|t|}{1+t^2}.$$
(4.13)

Observe here that λ is an even function so we are going to assume without loss of generality that t > 0. This being so, we write

$$\lambda(t) = \frac{h'(t)}{2h(t)} = \frac{1}{2} \frac{d}{dt} (\ln h(t))$$
$$\implies \ln h(t) = 2 \int_0^t \lambda(s) ds$$
$$\implies h(t) = e^{2 \int_0^t \lambda(s) ds}.$$

So we see there is a straight relation between λ and h. We can also rewrite (4.12) using (4.13) so that

$$\theta(x,t) = \frac{t}{1+t^2} \frac{|x|^2}{2} + \varphi(t), \quad t > 0.$$

The next step is to try to find ρ and φ . To do so we plug in (4.2) into Schrödinger's problem

$$\partial_t u = \frac{i}{2} \Delta u.$$

We see that

$$\partial_t u = (\partial_t \rho + i\rho \partial_t \theta) e^{i\theta},$$

and

$$\Delta u = (\Delta \rho + 2i\nabla \rho \cdot \nabla \theta + i\rho \Delta \theta - \rho |\nabla \theta|^2) e^{i\theta}.$$

If we plug these expressions in the equation and separate the real and imaginary parts we derive the following set of differential equations

$$\begin{cases} \partial_t \rho + \nabla \theta \cdot \nabla \rho + \frac{1}{2} \rho \Delta \theta = 0\\ \Delta \rho - \rho (2\partial_t \theta + |\nabla \theta|^2) = 0. \end{cases}$$
(4.14)

We solve the first differential equation using the method of characteristics. Since we are looking for the solution that minimizes the problem we use condition (4.10) and solve the first equation in (4.14). If we write it as an initial value problem we get

$$\begin{cases} \partial_t \rho + \lambda(t)x \cdot \nabla \rho + \frac{n}{2}\lambda(t)\rho = 0, \\ \rho(x,0) = g(x), \end{cases}$$

where $\rho = \rho(x,t)$ describes a surface. The goal is to write ρ as a collection of curves, which we name characteristic curves where each point is parametrized so that

$$(x,t) = (X(\tau,s), T(\tau,s)),$$

where τ and s are the parameters that we will define later.

First observe that the differential equation may be written as

$$(\partial_t \rho, \nabla_x \rho, -1) \cdot (1, \lambda x, -\frac{n}{2}\lambda \rho) = 0,$$

where the first vector is precisely the normal vector of the tangent plane at a given point (x, t). This means that the vector $(1, \lambda x, -\frac{n}{2}\lambda\rho)$ is orthogonal to the normal vector and hence contained inside the tangent plane. Observe further that this vector describes a curve along the surface ρ for each (x, t). This is precisely the characteristic curve. We want to parametrize this curve.

As the vector $(1, \lambda x, -\frac{n}{2}\lambda\rho)$ belongs to the tangent plane it satisfies the following relations

$$\frac{dt}{1} = \frac{dx_1}{\lambda x_1} = \dots = \frac{dx_n}{\lambda x_n} = \frac{d\rho}{-\frac{n}{2}\lambda\rho} = d\tau, \qquad (4.15)$$

where τ is the parameter defining the trajectory of the characteristic curves. Beside this, we need an extra parameter s that will tell us at which point of a given curve we are. Since we are on a n-dimensional space the parameter s will be a vector $s = (s_1, ..., s_n)$. Therefore we define as the initial characteristic curve ($\tau = 0$) the following:

$$\begin{cases} t(0,s) = 0\\ x_i(0,s_i) = s_i, \quad i = 1, ..., n\\ \rho(0,s) = g(s). \end{cases}$$
(4.16)

Now from (4.15) we see that

$$\begin{cases} t = \tau \\ x_i = c_i e^{\int_0^t \lambda(u) du} \\ \rho = c_0 e^{-\frac{n}{2} \int_0^t \lambda(u) du}, \end{cases}$$

where we use (4.16) to find the values of the constants c_i and c_0 so that

$$\begin{cases} c_i = s_i = x_i e^{-\int_0^t \lambda(u) du} \Longrightarrow s = x e^{-\int_0^t \lambda(u) du} \\ c_0 = g(s). \end{cases}$$
(4.17)

Gathering all the data we conclude that

$$\rho(x,t) = e^{-\frac{n}{2}\int_0^t \lambda(u)du} g\left(xe^{-\int_0^t \lambda(u)du}\right).$$
(4.18)

Observe that the function g is actually the initial data of Schrodinger's problem, i.e. the function u_0 . We also see that unlike the argument function θ , ρ does not need to be radial. Further, since we are assuming equality on (4.9) we can write (4.18) as

$$\rho(x,t) = (1+t^2)^{-n/4}g(x(1+t^2)^{-1/2}).$$

By solving the second differential equation in (4.14) we are going to determine what the initial data should be in order to minimize the problem (4.9). We are going to see that this differential equation may be reduced to the harmonic oscilator problem. First we talk about the 1-dimensional harmonic oscilator problem to see what the minimizers look like in that case and after we generalize it to dimensions n > 1.

4.2.1 The 1-dimensional harmonic oscilator

The time independent Schrödinger equation in dimension 1 may be written as

$$H\psi = E\psi, \tag{4.19}$$

where H is the Hamiltonian representing the energy (kinetic and potential) of the quantum system and E is a real number representing the energy level or eigenvalue. The function ψ is the eigenstate of the problem.

Making suitable changes equation (4.19) can be written as

$$-\psi''(y) + y^2\psi(y) = \gamma\psi(y).$$
(4.20)

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So we want to find the eigenstate ψ and the value γ attached to it. First observe that asymptotically when $|y| \to \infty$ equation (4.20) can be reduced to

$$\psi'' = y^2 \psi,$$

for the contribution of $\gamma \psi$ in that case would be negligible. The solution to this problem is given by

$$\psi(y) = H(y)e^{-y^2/2},\tag{4.21}$$

where H(y) are certain polynomials we calculate next. We may without loss of generality assume that H is a finite polynomial such that

$$H(y) = a_0 + a_1 y + \dots + a_p y^p$$
.

If we now plug (4.21) into (4.20) we obtain the following differential equation

$$-H''(y) + 2yH'(y) + (1-\gamma)H(y) = 0, \qquad (4.22)$$

from where we obtain the following recursive formula for the coefficients of the polynomial

$$a_{j+2} = \frac{2j+1-\gamma}{(j+2)(j+1)}a_j, \quad j \ge 0,$$
(4.23)

and in order to have a finite polynomial we impose as a condition that the numerator of the formula (4.23) is zero for certain j = k, thus

$$2k + 1 - \gamma = 0 \implies \gamma = 2k + 1.$$

The resulting polynomials from the procedure above turn out to be the well known Hermite polynomials, named after the French mathematician *Charles Hermite*. Some of them are,

$$H_0 = 1,$$

 $H_1 = 2y,$
 $H_2 = 4y^2 - 2,$
 $H_3 = 8y^3 - 12y.$
 \vdots

One of the properties of these polynomials is that they jump from even to odd as we go up the indexes and also that they form an orthogonal family. These polynomials may also be calculated by the following formula

$$H_k(x) = (-1)^k e^{x^2} \frac{d^k}{dx^k} e^{-x^2},$$
(4.24)

known as the Rodrigues formula thanks to the French mathematician *Benjamin Olinde Rodrigues*, who discovered this easy way to compute the polynomials.

Here is the graphic representation of the ones written above



We have thus found the eigenstates and eigenvalues of the problem, this is

$$\psi_k(y) = H_k(y)e^{-y^2/2}, \quad k = 0, 1, 2, \dots$$

and

$$\gamma_k = 2k + 1.$$

Now we go back to our problem and see how as we mentioned before the second equation in (4.14) may be reduced to the harmonic oscilator problem we just described. Indeed if we use (4.12) and (4.18) we see that

$$e^{-2\int_0^t \lambda(u)du}g'' - g(\lambda'(t)x^2 + 2\varphi'(t) + \lambda^2(t)x^2) = 0.$$

And if we rewrite the equation we have that

$$g'' - (\lambda'(t) + \lambda^2(t))x^2 e^{2\int_0^t \lambda(u)du} g = 2\varphi'(t)e^{2\int_0^t \lambda(u)du} g.$$
 (4.25)

Recall that we are assuming t > 0 and the definition of λ is explicit. This being so we can give a simpler representation of (4.25) as

$$g'' - (1+t^2)^{-1}x^2g = 2\varphi'(t)(1+t^2)g.$$
(4.26)

Now by making the following change of variables,

$$\tilde{x} \longmapsto (1+t^2)^{-1/2} x,$$

equation (4.26) becomes

$$g''(\tilde{x}) - \tilde{x}^2 g(\tilde{x}) = 2\varphi'(t)(1+t^2)g(\tilde{x}).$$
(4.27)

We can clearly identify now g as the eigenfunction of the problem so that

$$g_k(\tilde{x}) = H_k(\tilde{x})e^{-\tilde{x}^2/2}, \quad k = 0, 1, 2, \dots$$
 (4.28)

and,

$$\gamma_k = -2\varphi'(t)(1+t^2).$$

In particular for k=0 the eigenvalue attached to this solution is $\gamma_0=1$ so we get

$$-2\varphi'(t)(1+t^2) = 1,$$

from where we conclude

$$\varphi(t) = -\frac{1}{2}\arctan t.$$

All in all we see that at times where (4.10) is satisfied the solution to the differential equation system (4.14) in dimension 1 is given by

$$\rho(x,t) = (1+t^2)^{-1/4}g(x(1+t^2)^{-1/2}),$$

and,

$$\theta(x,t) = \frac{t}{1+t^2} \frac{x^2}{2} - \frac{\gamma_k}{2} \arctan t,$$

where γ_k are the eigenvalues of the harmonic oscilator and the initial data that minimizes (4.6) is given by

$$u_{0,k}(x) = H_k(x)e^{-x^2/2},$$

which are the Hermite functions.

Here is the graphic representation of some of the initial data



All computations above tell us that u is written as

$$u(x,t) = (1+t^2)^{-1/4} u_{0,k}(x(1+t^2)^{-1/2}) e^{i\left(\frac{t}{1+t^2}\frac{x^2}{2} - \frac{\gamma_k}{2}\arctan t\right)}.$$
(4.29)

Next we see that u is indeed a solution to (3.1).

$$e^{-i\theta}\partial_t u = -\frac{t}{2}(1+t^2)^{-5/4}u_{0,k} - xt(1+t^2)^{-7/4}u_{0,k}' + \frac{i}{2}(1+t^2)^{-9/4}x^2u_{0,k}' - \frac{i}{2}(1+t^2)^{-9/4}x^2t^2u_{0,k} - \frac{i}{2}\gamma_k(1+t^2)^{-5/4}u_{0,k},$$

and,

$$\frac{i}{2}e^{-i\theta}\partial_x^2 u = \frac{i}{2}(1+t^2)^{-5/4}u_{0,k}'' - xt(1+t^2)^{-7/4}u_{0,k}' - \frac{t}{2}(1+t^2)^{-5/4}u_{0,k} - \frac{i}{2}x^2t^2(1+t^2)^{-9/4}u_{0,k}.$$

From this we see that

$$e^{-i\theta} \left(\partial_t u - \frac{i}{2} \partial_x^2 u \right) = \frac{i}{2} (1+t^2)^{-9/4} x^2 u_{0,k} - \frac{i}{2} \gamma_k (1+t^2)^{-5/4} u_{0,k} - \frac{i}{2} (1+t^2)^{-5/4} u_{0,k}'' = \frac{i}{2} (1+t^2)^{-5/4} (-u_{0,k}'' + (1+t^2)^{-1} x^2 u_{0,k} - \gamma_k u_{0,k}) = \frac{i}{2} (1+t^2)^{-5/4} (-u_{0,k}'' + \tilde{x}^2 u_{0,k} - \gamma_k u_{0,k}).$$

The term inside the parenthesis on the right hand side is 0 since $u_{0,k}$ satisfies (4.20). We have thus proved that u is a solution of (3.1). Now we see that for the solution u (4.9) is indeed an equality. We compute

$$\begin{split} \int_0^t \left(\int_{\mathbb{R}} |\rho \nabla \theta|^2 dx \right)^{1/2} ds &= \int_0^t \left(\int_{\mathbb{R}} \frac{s^2}{(1+s^2)^{5/2}} |x|^2 |u_{0,k}(x(1+s^2)^{-1/2})|^2 dx \right)^{1/2} ds \\ &= \int_0^t \frac{s}{(1+s^2)^{5/4}} \left(\int_{\mathbb{R}} |x|^2 |u_{0,k}(x(1+s^2)^{-1/2})|^2 dx \right)^{1/2} ds \\ &= \int_0^t \frac{s}{\sqrt{1+s^2}} \left(\int_{\mathbb{R}} |y|^2 |u_{0,k}(y)|^2 dy \right)^{1/2} ds \\ &= a \int_0^t \frac{s}{\sqrt{1+s^2}} ds = a(\sqrt{1+t^2}-1). \end{split}$$

From where we get

$$a + \int_0^t \left(\int_{\mathbb{R}^n} |\rho \nabla \theta|^2 dx \right)^{1/2} ds = a + a(\sqrt{1 + t^2} - 1) = h(t)^{1/2},$$

just like we wanted to see.

The way we have defined the initial data in terms of Hermite functions suggests that there might be a relation between solutions. This is due to the fact that Hermite polynomials follow an iterative rule, say

$$H_k^{(j)}(x) = 2^j k(k-1) \cdots (k-j+1) H_{k-j}(x)$$

We are going to find a recursive formula for solutions u_k for which (4.6) is minimized.

We thus consider

$$u_{0,k}(x) = H_k(x)e^{-x^2/2},$$

and calculate the corresponding solution. First of all we compute the Fourier Transform of the given initial data,

$$\begin{split} (2\pi)^{1/2} \hat{u}_{0,k}(\xi) &= \int_{\mathbb{R}} e^{-ix\xi} H_k(x) e^{-x^2/2} dx = (-1)^k \int_{\mathbb{R}} e^{-ix\xi} e^{x^2} \frac{d^k}{dx^k} e^{-x^2} e^{-x^2/2} dx \\ &= (-1)^k \int_{\mathbb{R}} e^{-ix\xi} e^{x^2/2} \frac{d^k}{dx^k} e^{-x^2} dx \\ &= (-1)^{k-1} \int_{\mathbb{R}} (-i\xi) e^{-ix\xi} e^{x^2/2} \frac{d^{k-1}}{dx^{k-1}} e^{-x^2} dx \\ &+ (-1)^{k-1} \int_{\mathbb{R}} e^{-ix\xi} x e^{x^2/2} \frac{d^{k-1}}{dx^{k-1}} e^{-x^2} dx \\ &= (-i\xi) \int_{\mathbb{R}} e^{-ix\xi} (-1)^{k-1} e^{x^2} \frac{d^{k-1}}{dx^{k-1}} e^{-x^2} e^{-x^2} dx \\ &+ \int_{\mathbb{R}} e^{-ix\xi} x (-1)^{k-1} e^{x^2} \frac{d^{k-1}}{dx^{k-1}} e^{-x^2} e^{-x^2} dx \\ &= -i\xi \hat{u}_{0,k-1}(\xi) + \int_{\mathbb{R}} e^{-ix\xi} x u_{0,k-1}(x) dx \\ &= -i\xi \hat{u}_{0,k-1}(\xi) + i\partial_{\xi} \hat{u}_{0,k-1}(\xi). \end{split}$$

From here we can explicitly write the Fourier Transform of the solution, say

$$\hat{u}_k(\xi, t) = \hat{u}_{0,k}(\xi) e^{-\frac{i}{2}t\xi^2}$$

= $i \left(-\xi \hat{u}_{0,k-1}(\xi) + \partial_{\xi} \hat{u}_{0,k-1}(\xi)\right) e^{-\frac{i}{2}t\xi^2},$

and by the inversion formula of the Fourier transform we recover the solution,

$$(2\pi)^{1/2}u_k(x,t) = \int_{\mathbb{R}} e^{ix\xi} \hat{u}_k(\xi,t)d\xi$$

= $i \int_{\mathbb{R}} e^{ix\xi} (-\xi \hat{u}_{0,k-1}(\xi) + \partial_{\xi} \hat{u}_{0,k-1}(\xi))e^{-\frac{i}{2}t\xi^2}d\xi$
= $-i \int_{\mathbb{R}} e^{ix\xi} \xi \hat{u}_{0,k-1}(\xi)e^{-\frac{i}{2}t\xi^2}d\xi$
+ $i \int_{\mathbb{R}} e^{ix\xi} \partial_{\xi} \hat{u}_{0,k-1}(\xi)e^{-\frac{i}{2}t\xi^2}d\xi$
= $I_1 + I_2.$

We work on the second integral, I_2 ,

$$\begin{split} I_2 &= i \int_{\mathbb{R}} e^{ix\xi} \partial_{\xi} \hat{u}_{0,k-1}(\xi) e^{-\frac{i}{2}t\xi^2} d\xi \\ &= -i \int_{\mathbb{R}} ix e^{ix\xi} \hat{u}_{0,k-1}(\xi) e^{-\frac{i}{2}t\xi^2} d\xi - i \int_{\mathbb{R}} e^{ix\xi} \hat{u}_{0,k-1}(\xi) (-it\xi) e^{-\frac{i}{2}t\xi^2} d\xi \\ &= x \int_{\mathbb{R}} e^{ix\xi} \hat{u}_{0,k-1}(\xi) e^{-\frac{i}{2}t\xi^2} d\xi - t \int_{\mathbb{R}} e^{ix\xi} \xi \hat{u}_{0,k-1}(\xi) e^{-\frac{i}{2}t\xi^2} d\xi \\ &= x u_{k-1}(x,t) - t \int_{\mathbb{R}} e^{ix\xi} \xi \hat{u}_{0,k-1}(\xi) e^{-\frac{i}{2}t\xi^2} d\xi. \end{split}$$

So we have

$$u_k(x,t) = xu_{k-1}(x,t) - (i+t) \int_{\mathbb{R}} e^{ix\xi} \xi \hat{u}_{0,k-1}(\xi) e^{-\frac{i}{2}t\xi^2} d\xi$$

= $xu_{k-1}(x,t) - (i+t)I_3.$

Lastly we work out the integral I_3 so that,

$$I_{3} = -i \int_{\mathbb{R}} \nabla_{x} e^{ix\xi} \hat{u}_{0,k-1}(\xi) e^{-\frac{i}{2}t\xi^{2}} d\xi$$
$$= -i\partial_{x} \int_{\mathbb{R}} e^{ix\xi} \hat{u}_{0,k-1}(\xi) e^{-\frac{i}{2}t\xi^{2}} d\xi$$
$$= -i\partial_{x} u_{k-1}(x,t).$$

So we conclude

$$u_k(x,t) = xu_{k-1}(x,t) + (it-1)\partial_x u_{k-1}(x,t).$$
(4.30)

This recursive formula allows us to give explicit solutions for different initial data $u_{0,k}$ if we only know the first one of all, this is, $u_0(x,t)$. We proceed to calculate this first solution. The initial data attached to this solution is the Gaussian, say

$$u_{0,0}(x) = e^{-x^2/2},$$

for which

$$\hat{u}_{0,0}(\xi) = e^{-\xi^2/2}.$$

Using the Fourier Transform of the initial data we can thus define the Fourier Transform of the solution as

$$\hat{u}_0(\xi, t) = e^{-\xi^2/2} e^{-\frac{i}{2}t\xi^2}.$$

Therefore, the solution u_0 can be explicitly calculated,

$$(2\pi)^{1/2}u_0(x,t) = \int_{\mathbb{R}} e^{ix\xi} e^{-\xi^2/2} e^{-\frac{i}{2}t\xi^2} d\xi$$

= $\int_{\mathbb{R}} e^{ix\xi} e^{-\frac{|\xi|^2}{2}(1+it)} d\xi$
= $e^{-\frac{x^2}{2(1+it)}} \int_{\mathbb{R}} e^{-\frac{(1+it)}{2}\left(\xi-i\frac{x}{1+it}\right)^2} d\xi$
= $\frac{1}{\sqrt{1+it}} e^{-\frac{x^2}{2(1+it)}}.$

Or,

$$u_0(x,t) = \frac{1}{(1+t^2)^{1/4}} e^{-\frac{x^2}{2}\frac{1}{1+t^2}} e^{i\left(\frac{x^2}{2}\frac{t}{1+t^2} - \frac{1}{2}\arctan t\right)},$$

which agrees with the given ρ and θ .

Now we use this expression to get the second solution $u_1(x, t)$. From (4.30) we know that

$$u_1(x,t) = xu_0(x,t) + (it-1)\partial_x u_0(x,t).$$

We see that

$$\partial_x u_0(x,t) = -\frac{x}{(1+it)^{3/2}} e^{-\frac{x^2}{2(1+it)}},$$

so that

$$\begin{split} u_1(x,t) &= \frac{x}{(1+it)^{1/2}} e^{-\frac{x^2}{2(1+it)}} - (it-1)\frac{x}{(1+it)^{3/2}} e^{-\frac{x^2}{2(1+it)}} \\ &= \left(\frac{x(1+it)}{(1+it)^{3/2}} - \frac{x(it-1)}{(1+it)^{3/2}}\right) e^{-\frac{x^2}{2(1+it)}} \\ &= \frac{2x}{(1+it)^{3/2}} e^{-\frac{x^2}{2(1+it)}}. \end{split}$$

And if we write it in terms of the functions ρ and θ we have,

$$u_1(x,t) = \frac{2x}{(1+t^2)^{3/4}} e^{-\frac{x^2}{2(1+t^2)}} e^{i\left(\frac{x^2}{2}\frac{t}{1+t^2} - \frac{3}{2}\arctan t\right)}.$$

Here is a graphic representation of $|\rho|$,



Following up we can calculate the next solutions,

$$\begin{split} u_2(x,t) &= \frac{4x^2 - 2(1+t^2)}{(1+it)^{5/2}} e^{-\frac{x^2}{2(1+it)}}, \\ u_3(x,t) &= \frac{8x^3 - 12x(1+t^2)}{(1+it)^{7/2}} e^{-\frac{x^2}{2(1+it)}}, \\ u_4(x,t) &= \frac{16x^4 - 48x^2(1+t^2) + 12(1+t^2)^2}{(1+it)^{9/2}} e^{-\frac{x^2}{2(1+it)}}, \\ &\vdots \end{split}$$

It can be proved by induction that the general solution u_k can be written as

$$u_k(x,t) = \frac{P_k(x,(1+t^2))}{(1+it)^{\frac{2k+1}{2}}} e^{-\frac{x^2}{2(1+it)}}, \quad k = 0, 1, 2, \dots$$
(4.31)

where P_k is a real polynomial of degree k as the ones defined above.

4.2.2 The n-dimensional harmonic oscilator

We have seen that for dimension 1 everything works out fine and we were able to find the minimizers of (4.9) as the Hermite functions. However in the ndimensional problem the resolution of the harmonic oscilator needs a little more work, even though the outcome is still a polynomial function acting on the Gaussian as we see next. The problem has still the form

$$\Delta g + (2E - |x|^2)g = 0, \qquad (4.32)$$

where E is the energy which in our case is given by $2\varphi(t)(1+t^2)$.

We are not going to give all the details but sketch the idea of how the solution to the problem is gotten. The idea is to write it as a product of a radial function and an *angular* function defined on \mathbb{S}^{n-1} . We thus take $x = |x|\xi = r\xi$ where $\xi \in \mathbb{S}^{n-1}$. By making this change of variables we get

$$\Delta_x = \frac{\partial^2}{\partial r^2} + \frac{n-1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \Delta_{\xi}.$$
(4.33)

There exists a set of $\mathcal{N}(n, l)$ linearly independent spherical harmonics $S(\xi)$ which are polynomials of degree l in ξ such that

$$\Delta_{\xi}S + l(l+n-2)S = 0, \tag{4.34}$$

and the number $\mathcal{N}(n, l)$ is defined as

$$\mathcal{N}(n,l) = \begin{cases} \frac{(2l+n-2)(l+n-3)}{l!(n-2)!}, & l \ge 1\\ 1, & l = 0. \end{cases}$$

We consider now $g(x) = g(r\xi) = R(r)S(\xi)$ and by plugging (4.33) and (4.34) in (4.32) we get

$$\left[\frac{\partial^2}{\partial r^2} + \frac{n-1}{r}\frac{\partial}{\partial r} - \frac{l(l+n-2)}{r^2} + (2E-r^2)\right]R(r) = 0.$$
 (4.35)

By solving (4.35) we get the radial function

$$R(r) = c_{n,m,l} r^l e^{-r^2/2} L_m^{l+n/2-1}(r^2), \quad n > 1,$$
(4.36)

which belong to the energy eigenvalue $E = 2m + l + \frac{1}{2}n$ and where L_m^{α} are the mth order associated *Laguerre polynomials* which are the solution to the second order linear differential equation

$$xy'' + (\alpha + 1 - x)y' + my = 0,$$

where α is an arbitrary real number. This equation has nonsingular solutions only if *m* is a non-negative integer and the polynomial is given by the formula

$$L_m^{\alpha}(x) = \sum_{k=0}^m (-1)^k \frac{(m+\alpha)!}{(m-k)!(\alpha+k)!k!} x^k.$$
(4.37)

These polynomials may also be defined by a recursive formula, say

$$L_m^{\alpha}(x) = L_m^{\alpha+1}(x) - L_{m-1}^{\alpha+1}(x).$$

The first few associated Laguerre polynomials are

$$L_0^{\alpha}(x) = 1,$$

$$L_1^{\alpha}(x) = -x + \alpha + 1,$$

$$L_2^{\alpha}(x) = \frac{1}{2}[x^2 - 2(\alpha + 2)x + (\alpha + 1)(\alpha + 2)],$$

$$L_3^{\alpha}(x) = \frac{1}{6}[-x^3 + 3(\alpha + 3)x^2 - 3(\alpha + 2)(\alpha + 3)x + (\alpha + 1)(\alpha + 2)(\alpha + 3)]$$

And there is a relation between these polynomials and the ones by Hermite but only for $\alpha = -1/2$,

$$H_{2m}(x) = (-1)^m 2^{2m} m! L_m^{-1/2}(|x|^2),$$

$$H_{2m+1}(x) = (-1)^m 2^{2m+1} m! x L_m^{-1/2}(|x|^2).$$

All in all we see that the initial data for the minimizer of (4.9) are the eigenfunctions of the problem described above as $u_0(x) = u_0(r\xi) = R(r)S(\xi)$ where the functions R(r) are defined in (4.36) and $S = S(\xi)$ are spherical harmonics defined on the unit sphere. Moreover, the eigenvalues of the problem are given by $E = 2m + l + \frac{1}{2}n$ where m and l can take any non negative integer values so we see that

$$-2\varphi(t)(1+t^2) = E_{l,m,n} \Longrightarrow \varphi(t) = -\frac{E_{l,m,n}}{2} \arctan t.$$

From the last calculation we see that the argument does not change much for the n-dimensional problem. The minimizer can thus be defined as

$$u(x,t) = (1+t^2)^{-n/4} u_0(x(1+t^2)^{-1/2}) e^{i\left(\frac{t}{1+t^2}\frac{|x|^2}{2} - \frac{E_{l,m,n}}{2} \arctan t\right)}.$$
(4.38)

All the results obtained so far are gathered in the following theorem:

Theorem 4.2.1. Let u be a solution of Schrödinger's initial value problem 3.1 written as (4.2) and let h be defined as in (4.1). Then h satisfies the inequality (4.9) where $a^2 = h(0)$. Moreover if there is a time interval [0,T] with T > 0 such that equality is attained, then equality holds for every t and the solutions are given by

- 1. the family $\{u_k\}_{k\geq 0}$ defined in (4.31) if n = 1;
- 2. the solutions u defined in (4.38) if n > 1, where the initial data u_0 is given by

$$u_0(x) = u_0(r\xi) = R(r)S(\xi),$$

S are spherical harmonics defined on \mathbb{S}^{n-1} and R are defined in (4.36).

4.3 A minimizing problem for h_{δ}

The last section of this chapter is devoted to analyzing the same minimizing problem as the one of the previous section but for the function h_{δ} instead. We have seen that the minimizers for the problem are generated by the eigenfunctions of the harmonic oscilator problem, this is, Hermite functions. We will see that the same conclusion is reached in this case.

To do so we follow the same strategy as before. We are going to see that the computations does not change much. First we compute the derivative of h_{δ} ,

$$\begin{split} h_{\delta}'(t) &= \int_{\mathbb{R}^n} |x|^{2\delta} \partial_t |u(x,t)|^2 dx = 2Re \int_{\mathbb{R}^n} |x|^{2\delta} \bar{u} \partial_t u dx \\ &= Re \int_{\mathbb{R}^n} |x|^{2\delta} \bar{u} i \Delta u dx \\ &= -Im \int_{\mathbb{R}^n} |x|^{2\delta} \bar{u} \partial_t u dx \\ &= 2\delta Im \int_{\mathbb{R}^n} |x|^{2(\delta-1)} \bar{u} (x \cdot \nabla u) dx \\ &= 2\delta Im \int_{\mathbb{R}^n} |x|^{2\delta-1} \bar{u} \partial_r u dx, \end{split}$$

where $\partial_r u$ is the radial derivative of u.

At this point we use again the following definition of the solution u, say

$$u(x,t) = \rho(x,t)e^{i\theta(x,t)}.$$
(4.39)

If we now plug (4.39) into (3.9) and the expression of the derivative we just calculated, we have

$$h_{\delta}(t) = \int_{\mathbb{R}^n} |x|^{2\delta} \rho^2 dx, \qquad (4.40)$$

and

$$h_{\delta}'(t) = 2\delta \int_{\mathbb{R}^n} \rho^2 |x|^{2(\delta-1)} x \cdot \nabla \theta dx = 2\delta \int_{\mathbb{R}^n} \rho^2 |x|^{2\delta-1} \partial_r \theta dx.$$
(4.41)

Now we take the absolute value to the derivative and use Cauchy-Schwarz's inequality as we did before so that

$$\begin{aligned} |h_{\delta}'(t)| &\leq 2\delta \int_{\mathbb{R}^n} \rho^2 |x|^{2\delta-1} |\partial_r \theta| dx \\ &\leq 2\delta \left(\int_{\mathbb{R}^n} |x|^{2\delta} \rho^2 dx \right)^{1/2} \left(\int_{\mathbb{R}^n} |x|^{2\delta-2} \rho^2 |\partial_r \theta|^2 dx \right)^{1/2} \\ &= 2\delta h_{\delta}^{1/2}(t) \left(\int_{\mathbb{R}^n} |x|^{2\delta-2} \rho^2 |\partial_r \theta|^2 dx \right)^{1/2}, \end{aligned}$$

from where we have

$$\frac{|h_{\delta}'(t)|}{h_{\delta}^{1/2}(t)} \le 2\delta \left(\int_{\mathbb{R}^n} |x|^{2\delta-2} \rho^2 |\partial_r \theta|^2 dx \right)^{1/2}$$

Next we integrate both sides like we did for the case $\delta = 1$ so that

$$h_{\delta}^{1/2}(t) \le a_{\delta} + \delta \int_0^t \left(\int_{\mathbb{R}^n} |x|^{2\delta - 2} \rho^2 |\partial_r \theta|^2 dx \right)^{1/2} ds.$$

$$(4.42)$$

Our job is thus to find solutions minimizing this inequality. Nevertheless we see that the condition that minimizes this inequality is

$$\nabla \theta = \lambda(t)x$$

Using this and plugging it into the inequality above we have that

$$\begin{split} \frac{|h_{\delta}'(t)|}{h_{\delta}^{1/2}(t)} &= 2\delta\lambda(t)\left(\int_{\mathbb{R}^n} |x|^{2(\delta-1)}\rho^2 |x|^2 dx\right)^{1/2} \\ &= 2\delta\lambda(t)\left(\int_{\mathbb{R}^n} |x|^{2\delta}\rho^2 dx\right)^{1/2} \\ &= 2\delta\lambda(t)h_{\delta}^{1/2}, \end{split}$$

and hence,

$$\lambda(t) = \frac{1}{2\delta} \frac{|h_{\delta}'(t)|}{h_{\delta}(t)},$$

which coincides with the λ obtained for $\delta = 1$. We thus see how the conditions for a general $\delta \neq 1$ does not change.

Back to (4.42) we need to check that the integral on the right hand side is bounded. To do so, we recall that the second derivative of h_{δ} may be written as

$$h_{\delta}''(t) = -\frac{1}{4} \int_{\mathbb{R}^n} \Delta^2 \phi_{\delta}(x) |u(x,t)|^2 dx + \int_{\mathbb{R}^n} \nabla u D^2 \phi_{\delta} \overline{\nabla u} dx,$$

where $\phi_{\delta}(x) = |x|^{2\delta}$. We aim to prove that h_{δ} is convex so we need to see that the bilaplacian factor is negative in order to give a positive lower bound. If we thus compute the bilaplacian of the function ϕ_{δ} we see that

$$\begin{split} \Delta^2 \phi_{\delta}(x) &= -\frac{(n-1)(n-3)}{|x|^3} \phi' + \frac{(n-1)(n-3)}{|x|^2} \phi'' + \frac{2(n-1)}{|x|} \phi''' + \phi^{iv} \\ &= -\frac{(n-1)(n-3)}{|x|^3} 2\delta |x|^{2\delta-1} + \frac{(n-1)(n-3)}{|x|^2} 2\delta (2\delta-1) |x|^{2\delta-2} \\ &+ \frac{2(n-1)}{|x|} 2\delta (2\delta-1)(2\delta-2) |x|^{2\delta-3} + 2\delta (2\delta-1)(2\delta-2)(2\delta-3) |x|^{2\delta-4} \\ &= 2\delta (2\delta-2) |x|^{2(\delta-2)} \left((n-1)(n-3) + (2\delta-1)(2n+2\delta-5) \right). \end{split}$$

It is easy to see that this quantity is negative if $n \ge 3$ and $1/2 < \delta \le 1$. The case $\delta = 1/2$ gives also convexity but it is more complex and should be analyzed separately. Under these conditions we can write

$$h_{\delta}''(t) \ge \int_{\mathbb{R}^n} \nabla u D^2 \phi_{\delta} \overline{\nabla u} dx.$$

We need to rewrite the term inside the integral so that it is easier to manipulate. Observe that

$$\nabla u D^2 \phi_{\delta} \overline{\nabla u} = \phi_{\delta}'' |\partial_r u|^2 + \frac{\phi_{\delta}'}{r} |\nabla_\tau u|^2,$$

where ∂_r and ∇_{τ} are the radial and tangential derivatives respectively,

$$\nabla u = \frac{x}{|x|} \partial_r u + \nabla_\tau u,$$

with $\frac{x}{|x|} \nabla_{\tau} u = 0$. Hence taking $\phi_{\delta}(r) = r^{2\delta}$ for $1/2 < \delta \leq 1$ we see that

$$h_{\delta}''(t) \ge 2\delta(2\delta - 1) \int_{\mathbb{R}^n} |x|^{2(\delta - 1)} |\partial_r u|^2 dx$$

We now write the solution u as

$$u(x,t) = \rho(x,t)e^{i\theta(x,t)}, \quad \rho, \theta \in \mathbb{R},$$

so that

$$\partial_r u = (\partial_r \rho + i\rho \partial_r \theta) e^{i\theta}.$$

If we plug this expression into the one for h_{δ}'' we see that

$$h_{\delta}''(t) \ge 2\delta(2\delta - 1) \int_{\mathbb{R}^n} |x|^{2(\delta - 1)} |\partial_r u|^2 dx$$
$$= 2\delta(2\delta - 1) \int_{\mathbb{R}^n} |x|^{2(\delta - 1)} \rho^2 |\partial_r \theta|^2 dx$$

Observe that the last term is precisely the one we are trying to bound so we only need to check that h''_{δ} is bounded. Let $0 < T < \infty$, then

$$\frac{T}{2} \int_{-T/2}^{T/2} h_{\delta}''(t) dt \leq \int_{-T}^{T} (T - |t|) h_{\delta}''(t) dt$$
$$= \int_{-T}^{T} sgn(t) h_{\delta}'(t) dt = h_{\delta}(T) - h_{\delta}(-T),$$

which we know is bounded from the previous chapter, as we wanted to see.

Now that we know the bound in (4.42) is finite, we need to look for the minimizers of the problem as we did on the previous section. This job however does not change with respect to the case $\delta = 1$ since (4.14) is the same and the conditions on ρ and θ have not changed. Therefore the problem can be reduced again to the the harmonic oscilator problem and the solutions u minimizing (4.42) are given by (4.38). All results of this section are summed up in the following theorem, A minimizing problem for h_{δ}

Theorem 4.3.1. Let u be a solution of (3.1) written as (4.2) and h_{δ} be defined as in (3.9). If $1/2 < \delta < 1$ and $n \ge 3$ then h_{δ} satisfies (4.42) where $a_{\delta}^2 = h_{\delta}(0)$. Moreover if there is a time interval [0, T] with T > 0 such that equality is attained, then equality holds for every t and the solutions are given by u defined as in (4.38) where the initial data u_0 is given by

$$u_0(x) = u_0(r\xi) = R(r)S(\xi),$$

S are spherical harmonics defined on \mathbb{S}^{n-1} and R are defined in (4.36).

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