

university of groningen



faculty of science and engineering



mathematics and applied mathematics

Exact solutions to the time-dependent harmonic oscillator using Hermite polynomials

Bachelor's Project Applied Mathematics

January 2023

Student: I.C. van Vliet

First supervisor: Dr. A. Waters

Second assessor: Dr. J. Koellermeier

Abstract

In this paper, we consider time-dependent harmonic oscillators and construct a solution using Hermite polynomials. In this process, we use Gaussian wave packets. Using these solutions we can find observability constants for examples on $L^2(\mathbb{R}^2)$. In the first part, we will go over several topics needed for the final result. This includes the Fourier transform, the Schrödinger equation, Hermite polynomials and wave packets. In the second part, we introduce a lemma about the Fourier integral operator that helps us solve differential equations with timedependent operators with a quadratic potential and we find the observability constant for certain initial data.

Contents

1	Introduction	4
2	Background information	5
3	Fourier transform	7
	3.1 Multidimensional Fourier transform	. 10
	3.2 Fourier Integral Operator	. 11
4	Schrödinger equation	12
	4.1 Mathematical point of view	. 12
	4.2 Physicist's point of view	. 12
	4.3 Properties of the Schrödinger equation	. 13
	4.4 What about the Schrödinger equation with $ x ^2$. 15
5	Hermite polynomials and functions	16
	5.1 Use of Hermite polynomials in solving equations	. 19
	5.2 Multivariate Hermite polynomials	. 20
6	Wave packet for the Schrödinger equation	21
7	What is an observability inequality	24
8	Main result	26
9	Conclusion	30
	9.1 Future work	. 30

1 Introduction

This paper is based on the article Observability for Schrödinger equation with quadratic Hamiltonians by Alden Waters, [15]. In her paper, L^2 and $L^2 - L^{\infty}$ observability estimates on unbounded domains for a restricted class of initial data of time-dependent harmonic oscillators are proven. In this paper, we look at the case when the time-dependent harmonic oscillator is in \mathbb{R}^2 instead of \mathbb{R}^d . Our goal is to find exact solutions of the equation $i\partial_t u = \kappa_2 |x|^2 u + \Delta u$ using the Hermite polynomials. We will also give an example in \mathbb{R}^2 where we will compute the observability estimate of a certain set of initial data. For this to happen we first need to establish some definitions and give the reader the appropriate background information that is needed throughout the paper.

For this reason, we will start the paper by looking at the preliminary knowledge that is needed throughout the paper. We will go over the definition of an orthonormal basis, the definition of a norm in the $L^2(\mathbb{R}^2)$ space and the Hermitian inner product. We will also go over the Fourier series, the error function and the Gaussian integral.

In the next section, we remind the reader how the Fourier transform is constructed, the different forms of the Fourier transform that are used regularly and the definition of the Fourier transform in higher dimensions.

As our goal is to find a solution to a specific form of the Schrödinger equation, we introduce the Schrödinger equation and some properties of this very useful equation in section 4.

In section 5 we go over a certain type of the Schrödinger equation where we have a specific operator that includes a $|x|^2$ term. This makes is it so that we need a different well-posedness, which is given in this section. We also look at the Hamiltonian that can be associated with this very specific differential equation, which is $i\partial_t u = \kappa_2(t)|x|^2u + \Delta u$.

In section 6 we introduce what Hermite polynomials are. We also look at the Hermite functions and properties of both of these polynomials. We also explain why Hermite polynomials and Hermite functions can help us solve the differential equation with quadratic potential.

As we try to solve the differential equation that is a form of the Schrödinger equation, we need to have a look at wave packets as these often solve the Schrödinger equation. We go over what a wave packet is and look at the wave equation that we try to solve for specific initial data. We try to solve it by using the Fourier transform.

In an example for the solution of the time-dependent harmonic oscillator, we want to find the observability constant. To be able to do this, we define what an observability inequality and an observability constant are in section 8.

Finally, in section 9 we give an exact solution to the differential equation men-

tioned above. To be able to do this we use the Fourier integral operator. Using a specific form of initial data, we observe a specific form of a solution. With this solution, we can find the observability constant for this example with the chosen initial data.

2 Background information

The vectors v_1, v_2, \ldots, v_n form a basis for a vector space V if and only if they are linearly independent and they span V. An orthogonal basis for an inner product space is a basis for this space whose vectors are mutually orthogonal. An orthonormal basis is a normalized orthogonal basis. This means that a set $\{u_1, u_2, \ldots, u_n\}$ is orthonormal if and only if $\langle u_i, u_j \rangle = \delta_{ij}$ where

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

where δ_{ij} is called the Kronecker delta.

A Hilbert space H is a complete inner product space [11]. This means that it is a vector space that is equipped with an inner product and this inner product defines a distance function. Since the space has a distance function, Hilbert spaces are complete metric spaces.

An orthonormal system $\{a_k\}_{k\in B}$ is an orthonormal basis for a Hilbert space when the set is complete. This means that $\langle v, a_k \rangle = 0$ for all $k \in B$ and $v \in H$ then v = 0, where B is some index set.

The space $L^2(\mathbb{R}^2)$ denotes the set of square-integrable functions on \mathbb{R}^2 . This means that a function $f \in L^2(\mathbb{R}^2)$ satisfies

$$\int_{\mathbb{R}^2} |f|^2 dx < \infty$$

and it has the following norm

$$||f||_{L^2(\mathbb{R}^2)} = \left(\int_{\mathbb{R}^2} |f|^2 dx\right)^{\frac{1}{2}}$$

Furthermore, the space $L^2(\mathbb{R}^2)$ is a Hilbert space. The following properties hold for functions in a Hilbert space. We can take $f, g \in L^2(\mathbb{R}^2)$, so $||f||, ||g|| < \infty$ then by the triangle inequality, $||f + g|| \le ||f|| + ||g||$, we also have $||f + g|| < \infty$ and thus $f + g \in L^2(\mathbb{R}^2)$. For any complex constant c, we have ||cf|| = |c| ||f||and thus $cf \in L^2(\mathbb{R}^2)$. Hence we have that a Hilbert space is a complex vector space. The Cauchy-Schwarz inequality $|\langle f,g\rangle| \le ||f|| \, ||g||$ implies that the $L^2(\mathbb{R}^2)$ Hermitian inner product

$$\langle f,g \rangle = \int_{\mathbb{R}^2} f(x) \overline{g(x)} dx$$

of two square-integrable functions is well-defined and finite.

We want to define the Fourier series as was done in chapter 3 of [9]. The Fourier series of a function f(x) defined on $-l \le x \le l$ is

$$f(x) \sim \frac{a_0}{2} + \sum_{k=1}^{\infty} \left[a_k \cos\left(\frac{k\pi x}{l}\right) + b_k \sin\left(\frac{k\pi x}{l}\right)\right]$$

whose coefficients are given by the inner product formulae

$$a_{k} = \langle f, \cos(kx) \rangle = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(kx) dx \quad k = 0, 1, 2, 3, \dots$$
$$b_{k} = \langle f, \sin(kx) \rangle = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(kx) dx \quad k = 1, 2, 3, \dots$$

The Fourier series can be found for functions that, at the very least, have integrals in the coefficient formulae that are well-defined and finite. As convergences are not guaranteed and even when the infinite series converges it may not converge to the original function f(x), for this reason, we do not use the equal sign but the \sim sign.

The error function is a complex function of a complex variable defined as [16]

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$$

The complementary error function is closely related to the error function and is defined as

$$\operatorname{erfc}(z) = 1 - \operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_{z}^{\infty} e^{-t^2} dt$$

Furthermore, we have the complex error function which is given by

$$\operatorname{erfi}(z) = -i \operatorname{erf}(iz)$$

The Gaussian integral [18] is the integral of a Gaussian function given by $f(x) = e^{-x^2}$. The integral is

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

The integral of an arbitrary Gaussian function is

$$\int_{-\infty}^{\infty} e^{-ax^2 + bx + c} dx = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a} + c}$$

This is for the one-dimensional case. We can also find a Gaussian integral when the function is in \mathbb{R}^d namely

$$\int_{\mathbb{R}^d} e^{-a|x|^2} e^{i\xi \cdot x} dx = \left(\frac{\pi}{a}\right)^{\frac{d}{2}} e^{-\frac{|\xi|^2}{4a}}$$

3 Fourier transform

A Fourier transform is a mathematical transformation that decomposes functions depending on space or time into functions depending on spatial frequency or temporal frequency. It is a powerful mathematical tool for the analysis of aperiodic functions. One of the most important properties of the Fourier transform is that it converts calculus, differentiation and integration, into algebra, multiplication and division. [9]

Let f(x) be a function defined for $-\infty < x < \infty$. The goal is to construct a Fourier expansion for f(x) in terms of basic trigonometric functions.

We begin by taking the re-scaled Fourier series on a symmetric interval [-l, l] of length 2l, which is

$$f(x) \sim \sum_{k=-\infty}^{\infty} c_k e^{ik\pi x/l}$$
 where $c_k = \frac{1}{2l} \int_{-l}^{l} f(x) e^{-ik\pi x/l}$

We can rewrite this in the adapted form

$$f(x) \sim \sum_{\nu = -\infty}^{\infty} \sqrt{\frac{\pi}{2}} \frac{\widehat{f}_l(k_{\nu})}{l} e^{ik_{\nu}x}$$

We take the sum over the frequencies $k_{\nu} = \frac{\pi\nu}{l}$, $\nu = 0, \pm 1, \pm 2, \ldots$, where the frequencies are discrete. These frequencies correspond to the trigonometric functions that have period 2*l*. The Fourier coefficients can now be denoted by

$$c_{k} = \frac{1}{2l} \int_{-l}^{l} f(x) e^{-ik_{\nu}x} dx = \sqrt{\frac{\pi}{2}} \frac{\widehat{f}_{l}(k_{\nu})}{l}$$

so that

$$\widehat{f}_l(k_\nu) = \frac{1}{\sqrt{2\pi}} \int_{-l}^{l} f(x) e^{-ik_\nu x} dx$$

Reformulating the formula of the basic Fourier series allows us to pass to the limit as the length of the interval $l \to \infty$. On an interval of 2l, a function in Fourier series form can be represented by the frequencies k_{ν} , where the required k_{ν} are equally distributed. The interfrequency spacing is $\Delta k = k_{\nu+1} - k_{\nu} = \frac{\pi}{l}$. As $l \to \infty$, the spacing $\Delta k \to 0$, which means that the relevant frequencies become more and more densely packed in the line $-\infty < k < \infty$. When we take $l \to \infty$ we expect that all possible frequencies will be represented. We see that by letting $k_{\nu} = k$ be arbitrary and sending $l \to \infty$, we obtain the following integral with infinite endpoints

$$\widehat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

which is known as the Fourier transform of the function f(x). If f(x) is piecewise continuous and decaying to 0 reasonably quickly as $|x| \to \infty$, its Fourier transform $\widehat{f}(k)$ is defined for all possible frequencies $k \in \mathbb{R}$. The Fourier transform is often abbreviated as $\widehat{f}(k) = \mathcal{F}[f(x)]$, where \mathcal{F} is the Fourier transform operator. This operator maps each function of the spatial variable x to a function of the frequency variable k.

We can also use the Fourier transform to reconstruct the original function, which follows a similar limiting procedure. We apply this limiting procedure to the Fourier series, but we first rewrite this in a more suggestive form

$$f(x) \sim \frac{1}{\sqrt{2\pi}} \sum_{\nu = -\infty}^{\infty} \widehat{f}_l(k_\nu) e^{ik_\nu x} \Delta k$$

where Δk is as defined above. For each fixed value of x, the right-hand side has the form of a Riemann sum approximating the integral

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\widehat{f}_l(k)e^{ikx}dk$$

As $l \to \infty$, $\hat{f}_l(k_{\nu})$ converge to the Fourier transform: $\hat{f}_l(k) \to \hat{f}(k)$. The interfrequency spacing $\Delta k = \frac{\pi}{l} \to 0$. From this we expect the Riemann sum to converge to the limiting integral

$$f(x) \sim \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widehat{f}(k) e^{ikx} dk$$

This formula is the inverse Fourier transform and is denoted by $f(x) = \mathcal{F}^{-1}[\widehat{f}(k)]$. It is used to recover the original formula from its Fourier transform.

We have seen one form of the Fourier transform above, but there are two more forms that are commonly used. The form we have been using up to now is called the unitary form for angular frequency. We also have a non-unitary form for angular frequency which is as follows

$$\hat{g}(\xi) = \int_{-\infty}^{\infty} g(x) e^{-i\xi x} dx$$

The angular frequency is given by $\xi = 2\pi\omega$, where ω is the ordinary frequency. We see that when we substitute this into our Fourier transform we obtain a third form namely the unitary form for ordinary frequency which is as follows

$$\hat{h}(\omega) = \int_{-\infty}^{\infty} h(x) e^{-2\pi i \omega x} dx$$

These forms are similar to each other in the following sense

$$\hat{f}(\xi) = \frac{1}{\sqrt{2\pi}} \hat{h}(\frac{\xi}{2\pi}) = \frac{1}{\sqrt{2\pi}} \hat{g}(\xi)$$

Each of these forms has an inverse Fourier transform as well. These are given by

$$g(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{g}(\xi) e^{i\xi x} d\xi$$
$$h(x) = \int_{-\infty}^{\infty} \hat{h}(\omega) e^{2\pi i\omega x} d\omega$$

Both the Fourier and the inverse Fourier transform define linear operators on function space. The following holds:

$$\mathcal{F}[f(x) + g(x)] = \mathcal{F}[f(x)] + \mathcal{F}[g(x)] = \widehat{f}(k) + \widehat{g}(k)$$
$$\mathcal{F}[cf(x)] = c\mathcal{F}[f(x)] = c\widehat{f}(k)$$

We can also take the Fourier transform of derivatives of the function. We make a distinction between spatial derivatives and derivatives with respect to time. This will be useful later on when we want to find the Fourier transform of the wave equation. We first show how to take the Fourier transform of a derivative with respect to time, where we use what was done in [4].

$$\begin{aligned} \mathcal{F}[\frac{\mathrm{d}}{\mathrm{d}t}u(t,x)] &= \int_{-\infty}^{\infty} \frac{\mathrm{d}}{\mathrm{d}t}u(t,x)e^{-i\xi x}dx \\ &= \int_{-\infty}^{\infty} \lim_{h \to 0} \frac{u(t+h,x) - u(t,x)}{h}e^{-i\xi x}dx \\ &= \lim_{h \to 0} \frac{1}{h} \int_{-\infty}^{\infty} u(t+h,x)e^{-i\xi x} - u(t,x)e^{-i\xi x}dx \\ &= \lim_{h \to 0} \left[\hat{u}(t+h,\xi) - \hat{u}(t,\xi)\right] \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\hat{u}(t,\xi) \end{aligned}$$

The Fourier transform of the spatial derivatives can be found using integration by parts in the following way

$$\mathcal{F}\left[\frac{\mathrm{d}}{\mathrm{d}x}u(t,x)\right] = \int_{-\infty}^{\infty} \frac{\mathrm{d}}{\mathrm{d}x}u(t,x)e^{-i\xi x}dx$$
$$= u(t,x)e^{-i\xi x}\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} u(t,x)(-i\xi)e^{-i\xi x}dx$$
$$= i\xi \int_{-\infty}^{\infty} u(t,x)e^{-i\xi x}dx$$
$$= i\xi \mathcal{F}[u(t,x)]$$

We can use induction on this process to obtain the following

$$\mathcal{F}[\frac{\mathrm{d}^n}{\mathrm{d}x^n}u(t,x)] = (i\xi)^n \mathcal{F}[u(t,x)]$$

Now that we know what a Fourier transform is we want to show that the Fourier transform of a Gaussian function is again a Gaussian function. To do this we take $f(x) = e^{-x^2}$ and take the Fourier transform

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} e^{-x^2 - i\xi x} dx$$
$$= \sqrt{\pi} e^{-\frac{|\xi|^2}{4}}$$

where we have used the Gaussian integral.

3.1 Multidimensional Fourier transform

Up to now, we have looked at the one-dimensional Fourier transform. We can expand this theory to higher dimensions. This is done in the following way. We can take the Fourier transform of a function $f \in L^2(\mathbb{R}^d)$, where the Fourier transform is defined as

$$\hat{f}(\xi) = \frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\mathbb{R}^d} f(x) e^{-ix \cdot \xi} dx$$

where $x \cdot \xi = x_1 \xi_1 + x_2 \xi_2 + \ldots + x_d \xi_d$, which is the standard inner product between x and ξ . This multidimensional Fourier transform also has an inverse which is given by

$$f(x) = \frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \hat{f}(\xi) e^{ix \cdot \xi} d\xi$$

We have seen that there are multiple forms of the one-dimensional Fourier transform. This is also true for the multidimensional Fourier transform. There are again two more forms that are commonly used [17]. These are given by

$$\hat{g}(\xi) = \int_{\mathbb{R}^n} g(x) e^{-i\xi \cdot x} dx$$
$$\hat{h}(\omega) = \int_{\mathbb{R}^n} h(x) e^{-2\pi i\omega \cdot x} dx$$

with corresponding inverses

$$g(x) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \hat{g}(\xi) e^{i\xi x} d\xi$$
$$h(x) = \int_{\mathbb{R}^n} \hat{h}(\omega) e^{2\pi i\omega x} d\omega$$

3.2 Fourier Integral Operator

The Fourier integral operator is an important tool in the theory of partial differential equations, which is looked at in chapter 3 of [8]. A Fourier integral operator T is given by

$$(Tf)(x) = \int_{\mathbb{R}^n} e^{2\pi i \Phi(x,\xi)} a(x,\xi) \widehat{f}(\xi) d\xi$$

where \hat{f} denotes the Fourier transform of f, $a(x,\xi)$ is a standard symbol which is compactly supported in x and Φ is real valued. A standard symbol is a polynomial representing a differential operator. We also have that $\det\left(\frac{\partial^2 \Phi}{\partial x_i \partial \xi_i}\right) \neq 0$ on the support of a.

4 Schrödinger equation

The Schrödinger equation is a differential equation that governs the behaviour of wave functions [5]. A wave function is a solution to the Schrödinger equation. It is a mathematical function and it relates the position of an electron at a certain point to the amplitude of its wave, which corresponds to its energy. This means that each wave function is associated to a potential energy E. By the superposition principle, we can add wave functions and multiply them by a complex number to obtain a new wave function and form a Hilbert space.

There are multiple forms of the Schrödinger equation namely, from a mathematical and physicist's point of view, the time-dependent Schrödinger equation and the time-independent Schrödinger equation.

4.1 Mathematical point of view

The abstract form of the Schrödinger equation is, as defined in chapter 9 of [9]

$$i\hbar\frac{\partial\psi}{\partial t} = S[\psi]$$

where S is a linear operator of the form $S = L^* \circ L$. This operator is either positive definite, when ker $L = \{0\}$, or positive semi-definite, when $0 \neq v \in \ker L = \ker S$. This operator is also self-adjoint, which means that it is its own adjoint. The adjoint S^* of the operator satisfies

$$\langle Sx, y \rangle = \langle x, S^*y \rangle$$

An operator is thus self-adjoint when $S = S^*$. This form of the Schrödinger equation is from a mathematical point of view.

4.2 Physicist's point of view

The following equation is how Erwin Schrödinger defined the Schrödinger equation in 1926,

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$$

where \hbar is the reduced Planck constant, which is the original Planck's constant divided by 2π , and \hat{H} is the Hamiltonian operator [5]. The Hamiltonian operator is defined by $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V$ where *m* is the mass of the particle and V(x,t) is the potential that represents the environment in which the particle exists. Here we see that the linear operator S is defined as the Hamiltonian operator, which is how we can relate the mathematical point of view to the physicist's point of view.

4.3 Properties of the Schrödinger equation

At each time t, the solution $\psi(t, x)$ to the Schrödinger equation represents the wave function of the quantum system. It should be a complex-valued, square-integrable function having unit L^2 norm, $\|\psi\| = 1$.

Proposition 1 If $\psi(t, x)$ is a solution to the Schrödinger equations, its Hermitian L^2 norm $||\psi(t, \cdot)||$ is fixed for all time.

The proof of this proposition can be found in chapter 9 of [9].

If the initial data $\psi(t_0, x) = \psi_0(x)$ is a wave function, with $||\psi_0|| = 1$, then, at each time t, the solution $\psi(t, x)$ to the Schrödinger equation has norm 1 as well. This means that throughout the evolutionary process, the solution $\psi(t, x)$ remains a wave function.

One of the spectral theorems states that a compact self-adjoint operator on a Hilbert space can be diagonalized. This also means that there is an orthonormal basis for this Hilbert space that consists of the eigenvectors of the operator and the eigenvalues of the operator are real. This is why we can use spectral decomposition to find a solution to the Schrödinger equation.

The Schrödinger equation looks similar to a diffusion equation. With this information, we can seek separable solutions with an exponential ansatz: $\psi(t, x) = e^{\alpha t}v(x)$. Substituting this expression into the Schrödinger equation and cancelling common exponential factors reduces the problem to the usual eigenvalue problem $S[v] = \lambda v$, with eigenvalue $\lambda = i\hbar\alpha$. Using the fact that S is self-adjoint and the eigenvalues have to be real, by the spectral theorem mentioned above. Let v_k denote the normalized eigenfunction, so $||v_k|| = 1$, associated with the k^{th} eigenvalue λ_k . The complex-valued function $\psi_k(t, x) = e^{-i\lambda_k t/\hbar}v_k(x)$ is the corresponding eigensolution of the Schrödinger equation. We observe that the eigensolutions of the Schrödinger equation are periodic, where the frequencies are $\omega_k = -\lambda_k/\hbar$. The frequencies are vibrational and also proportional to the eigenvalues. The general solution is the periodic series in the fundamental eigensolutions,

$$\psi(t,x) = \sum_{k} c_k \psi_k(t,x) = \sum_{k} c_k e^{-i\lambda_k t/\hbar} v_k(x)$$

whose coefficients are specified by the initial conditions. The Schrödinger equation

is well-posed in the past which is implied by the periodicity of the summands. This means we can determine both the past and future behaviour of a quantum system from its present form.

The eigenvalues represent the energy levels of the system described by the Schrödinger equation and can be experimentally detected by exciting the system.

The term Schrödinger equation actually refers to two types of equations, namely the time-dependent Schrödinger equation which describes how a wave function evolves over time, and the time-independent Schrödinger equation, which is an equation of state for wave functions of definite energy [12]. We will first look at the time-dependent Schrödinger equation.

The state of a particle at a time t is described by a wave function, which in this case is a complex-valued function $\psi(t) : \mathbb{R}^d \to \mathbb{C}$ which is normalized such that $\langle \psi(t), \psi(t) \rangle = 1$ holds. As we have seen before, we denote the inner product by \langle , \rangle which is defined by

$$\langle \phi, \psi \rangle := \int_{\mathbb{R}^d} \phi(q) \overline{\psi(q)} dq$$

A wave function $\psi(t)$ does have an average position $\langle q(t) \rangle$, defined as

$$\langle q(t) \rangle := \langle Q\psi(t), \psi(t) \rangle = \int_{\mathbb{R}^d} q |\psi(t,q)|^2 dq$$

where the position operator Q is the operation of multiplication by q, which means that $Q\psi(t,q) := q\psi(t,q)$. It also has an average momentum $\langle p(t) \rangle$ defined as

$$\langle p(t) \rangle := \langle P\psi(t), \psi(t) \rangle = \frac{\hbar}{i} \int_{\mathbb{R}^d} (\nabla_q \psi(t,q)) \overline{\psi(t,q)} dq$$

where the momentum operator P is defined by Planck's law

$$P\psi(t,q) := \frac{\hbar}{i} \nabla_q \psi(t,q)$$

The vector $\langle p(t) \rangle$ is a real-valued vector because all the components of P are selfadjoint.

This gives us the time-dependent Schrödinger equation $i\hbar \frac{\partial \psi}{\partial t} = H\psi$, where $H = \frac{|P|^2}{2m} + V(Q)$. We have that V(q) represents the potential energy of the particle.

In other words, we have

$$i\hbar\frac{\partial\psi}{\partial t}(t,q) = -\frac{\hbar^2}{2m}\Delta_q\psi(t,q) + V(q)\psi(t,q)$$

where $\Delta_q \psi$ is the Laplacian of ψ . We can normalize this equation as $\hbar = m = 1$ and write x instead of q, and we can now write the Schrödinger equation in the form $i \frac{\partial \psi}{\partial t}(t, x) = -\Delta_x \psi(t, x) + V(x)\psi(t, x)$.

We will now look at the time-independent Schrödinger equation. It is possible that the quantum state ψ oscillates in time according to the formula $\psi(t,q) = e^{\frac{E}{i\hbar}t}\psi(0,q)$ for some real number E. If this holds, it is true that $H\psi(t) = E\psi(t)$ for all times t, and this is known as the time-independent Schrödinger equation. E is referred to as the energy level or the eigenvalue of the state ψ . In general ψ does not have a simple oscillation behaviour in time but is instead a superposition or linear combination of such oscillating states.

4.4 What about the Schrödinger equation with $|x|^2$

The Schrödinger equation with an $|x|^2$ term can be realized by using a class of time-dependent quadratic operators of the following form

$$L = -\kappa_1(t)\Delta + \kappa_2(t)|x|^2$$

where $0 \leq \kappa_2(t)$ depends continuously on time t for $0 \leq t \leq T$, we also assume that $\kappa_1(t)$ is bounded below by a positive constant and $\kappa_1 \in \mathcal{C}^1([0,T])$.

Using this time-dependent quadratic operator we can write

$$\frac{\partial}{\partial t}u(t,x) + iLu(t,x) = 0 \quad 0 < t \le T, \quad x \in \mathbb{R}^d$$

with initial condition $u_0 = u(0, x)$. The term $|x|^2$ is non $L^2(\mathbb{R}^d)$, and because of this, we need a different definition of well-posedness, which is defined as in [10] and [15]. We can set

$$B = \{ u \in L^2(\mathbb{R}^d) : x^{\alpha} D_x^{\beta} u \in L^2(\mathbb{R}^d), \alpha, \beta \in \mathbb{N}_0^d, |\alpha + \beta| \le 2 \}$$

The space B is a Hilbert space equipped with the norm

$$\|u\|_B^2 = \sum_{\substack{\alpha,\beta \in \mathbb{N}_0^d, \\ |\alpha+\beta|=2}} \left\| x^{\alpha} D_x^{\beta} u \right\|_{L^2(\mathbb{R}^d)}^2$$

To this partial differential equation, we can associate the following Hamiltonian

$$H = \kappa_1(t)|p|^2 + \kappa_2(t)|x|^2$$

where $\kappa_1(t), \kappa_2(t)$ are continuous functions. The Hamiltonian trajectories are the solution (x(t), p(t)) to

$$\frac{\mathrm{d}x_i(t)}{\mathrm{d}t} = 2\kappa_1(t)p_i(t) \quad \frac{\mathrm{d}p_i(t)}{\mathrm{d}t} = -2\kappa_2(t)x_i(t) \quad i = 1,\dots,d \quad 0 \le t \le T$$

with (x(0), p(0)) such that x(0) = (1, ..., 1), p(0) = (0, ..., 0). It is non-zero if for all times t, $0 \le t \le T$ if $x_i(t) \ne 0$ for all i = 1, ..., d and the quantity

$$a(t) = e^{-\int_0^t \frac{p_i(s)\kappa_1(s)}{x_i(s)}ds}$$

is bounded. This quantity is the amplitude of a one-dimensional wave packet. This definition can be found in section 2 of [15], where it is definition 2.

5 Hermite polynomials and functions

As is done in chapter 18 of [1] we will give an overview of the Hermite polynomials, Hermite functions and its most important properties. The Hermite polynomials are given by

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$$

The Hermite polynomials are orthogonal with respect to the function $w(x) = e^{-x^2}$. This means that

$$\int_{-\infty}^{\infty} H_m(x)H_n(x)w(x)dx = 0$$

for all $m \neq n$. Furthermore, we have

$$\int_{-\infty}^{\infty} H_m(x)H_n(x)w(x)dx = 2^n n! \sqrt{\pi}\delta_{mn}$$

where δ_{mn} is the Kronecker delta.

The first six Hermite polynomials are given by

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

$$H_2(x) = 4x^2 - 2$$

$$H_3(x) = 8x^3 - 12x$$

$$H_4(x) = 16x^4 - 48x^2 + 12$$

$$H_5(x) = 32x^5 - 160x^3 + 120x$$

We can put these polynomials in a graph to get a better idea of what they look like.



Figure 1: The first six Hermite polynomials [19]

Using the Hermite polynomials we can define the Hermite functions in the following way

$$h_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) e^{-\frac{x^2}{2}}$$

which is a normalization of the Hermite polynomials. We have seen that the Hermite polynomials are orthogonal with respect to the weight function $w(x) = e^{-x^2}$, so by normalizing these we have that the Hermite functions are an orthonormal basis for the Hilbert space $L^2(\mathbb{R}^2)$. We can show that

$$\int_{-\infty}^{\infty} h_m(x)h_n(x)dx = \delta_{mn}$$

The first six Hermite functions are given by

$$\begin{split} h_0(x) &= \pi^{-\frac{1}{4}} e^{-\frac{1}{2}x^2} \\ h_1(x) &= \sqrt{2}\pi^{-\frac{1}{4}} x e^{-\frac{1}{2}x^2} \\ h_2(x) &= (\sqrt{2}\pi^{\frac{1}{4}})^{-1} (2x^2 - 1) e^{-\frac{1}{2}x^2} \\ h_3(x) &= (\sqrt{3}\pi^{\frac{1}{4}})^{-1} (2x^3 - 3x) e^{-\frac{1}{2}x^2} \\ h_4(x) &= (2\sqrt{6}\pi^{\frac{1}{4}})^{-1} (4x^4 - 12x^3 + 3) e^{-\frac{1}{2}x^2} \\ h_5(x) &= (2\sqrt{15}\pi^{\frac{1}{4}})^{-1} (4x^5 - 20x^3 + 15x) e^{-\frac{1}{2}x^2} \end{split}$$



Figure 2: The first six Hermite functions [19]

We can also find the exponential generating function of the Hermite polynomials, as is done in [13]. This is given by

$$g(x,t) = e^{-t^2 + 2tx} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!}$$

Using the exponential generating function we can find the recurrence relation in the following way

$$\frac{\partial}{\partial t}g(x,t) = (-2t + 2x)e^{-t^2 + 2tx} = \sum_{n=0}^{\infty} H_{n+1}(x)\frac{t^n}{n!}$$

We can expand the terms and put in the generating function again to obtain

$$-2\sum_{n=0}^{\infty}H_n(x)\frac{t^{n+1}}{n!} + 2x\sum_{n=0}^{\infty}H_n(x)\frac{t^n}{n!} = \sum_{n=1}^{\infty}H_n(x)\frac{t^{n-1}}{(n-1)!}$$

Relabeling this equation and equating the coefficients of t^n gives the following recurrence relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \text{ for } n \ge 1$$

Using a similar trick we can also find the derivative of the Hermite polynomial. This time we differentiate the generating function with respect to x instead of t to obtain

$$\frac{\partial}{\partial x}g(x,t) = 2te^{-t^2 + 2tx} = \sum_{n=0}^{\infty} H'_n(x)\frac{t^n}{n!}$$

Plugging into the generating function we get

$$2\sum_{n=0}^{\infty} H_n(x) \frac{t^{n+1}}{n!} = \sum_{n=1}^{\infty} H_n(x) \frac{t^n}{n!}$$

Relabeling and equating the coefficients of t^n gives

$$H'_n(x) = 2nH_{n-1}(x) \quad \text{for } n \neq 1$$

From these two facts, we can derive the Hermite differential equation. Combining

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$$
 and $H'_n(x) = 2nH_{n-1}(x)$

gives us

$$H_{n+1}(x) = 2xH_n(x) - H'_n(x)$$

To obtain the Hermite differential equation, we differentiate the equation above with respect to x to obtain

$$H'_{n+1}(x) = 2H_n(x) + 2xH'_n(x) - H''_n(x)$$

rewriting this gives us

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0$$

which is how the Hermite differential equation is obtained. As can be expected, the Hermite polynomials are solutions to the Hermite differential equation.

5.1 Use of Hermite polynomials in solving equations

There are multiple reasons why the Hermite polynomials are interesting and useful. In this section, we give a short overview of how the Hermite polynomials can help us solve the Schrödinger equation.

First of all, the Hermite functions are the eigenfunctions of the Fourier transform. This can be seen in the following way

$$\mathcal{F}[h_n(x)](k) = \widehat{h_n}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ixk} h_n(x) dx = (-i)^n h_n(k)$$

This means that they satisfy $\mathcal{F}(h_n(x)) = (-i)^n h_n(x)$. Here we can see the relation between the Fourier transform and the Hermite functions.

Another way that Hermite polynomials and Hermite functions can help us solve the equation is in the following way. After we normalize the Hermite polynomials into the Hermite functions, we have the Hermite differential equation in terms of Hermite functions, namely as

$$h_n''(x) + (2n+1-x^2)h_n(x) = 0$$

This equation is equivalent to the Schrödinger equation for the harmonic oscillators. This means that Hermite functions are eigenfunctions of this specific Schrödinger equation.

We can also look at the simple harmonic oscillator [3]. First, we recall the timeindependent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

where m is the particle mass and E is its energy. We obtain the simple harmonic oscillator when $V(x) = \frac{1}{2}m\omega^2 x^2$ and the Schrödinger equation becomes

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + \left(-\frac{m^2\omega^2}{\hbar^2}x^2 + \frac{2mE}{\hbar^2}\right)\psi(x) = 0$$

This looks very similar to the Hermite equation in terms of Hermite functions. The Hermite functions are solutions of the simple harmonic oscillator. They are also the eigenfunctions of the simple harmonic oscillator when $\hbar = m = 1$.

5.2 Multivariate Hermite polynomials

We can extend all this theory to multivariate Hermite polynomials, like is done in [multivariableHermite]. Before we do this we recall the multi-index notation: a d-dimensional multi-index is a d-tuple $\mathbf{k} = (k_1, \ldots, k_d)$ with nonnegative integer entries. We have the following properties for $\mathbf{k}, \mathbf{j} \in \mathbb{N}_0^d$ and $\mathbf{x} \in \mathbb{R}^d$:

- $\mathbf{k} \leq \mathbf{j} \Leftrightarrow k_i \leq j_i \text{ for all } i = 1, \dots, d$
- $\mathbf{k} + \mathbf{j} = (k_1 + j_1, \dots, k_d + j_d)$
- $|\mathbf{k}| = k_1 + \dots + k_d$
- $\mathbf{k}! = k_1! \cdots k_d!$
- $\mathbf{x}^{\mathbf{k}} = x_1^{k_1} \cdots x_d^{k_d}$

We can now define the multivariate Hermite polynomial $H_{\mathbf{k}}(\mathbf{x})$ with $\mathbf{x} \in \mathbb{R}^d$ as

$$H_{\mathbf{k}}(\mathbf{x}) = \prod_{j=1}^{d} H_{k_j}(x_j)$$

The exponential generating function G of the Hermite polynomials is given by

$$G(\mathbf{x}, \mathbf{t}) := e^{2\mathbf{x}^{\top}}\mathbf{t} - \mathbf{t}^{\top}\mathbf{t} = \sum_{\mathbf{k} \in \mathbb{N}_0^d} H_{\mathbf{k}}(\mathbf{x}) \frac{\mathbf{t}^{\mathbf{k}}}{\mathbf{k}!}$$

with $\mathbf{x}, \mathbf{t} \in \mathbb{R}^d$.

6 Wave packet for the Schrödinger equation

We have to start by understanding what a wave packet is before we can look at the wave packet for the Schrödinger equation.

We know that when solving a wave equation it is possible that there are multiple solutions to this equation. The superposition principle states that when there are multiple solutions to the wave equation, the sum of the solutions is also a solution to the wave equation. A wave packet is a combination of component waves. This means that a wave packet can be analyzed into an infinite set of sinusoidal waves of different frequencies, with phases and amplitudes such that they interfere constructively over a small portion of space and destructively elsewhere.



Figure 3: Wave packet[20]

Now that we have an idea of what a wave packet is in words, let us have a look at wave packets from a mathematical perspective, as is done in [2]. First, we define a plane wave as the following function

$$\psi(t,x) = Ae^{i(kx - \omega t)}$$

where A is the amplitude of the wave, k is the wave number and ω is the angular frequency. When A, k and ω are constants, plane waves are solutions of the wave equation

$$\frac{\partial^2 \psi(t,x)}{\partial t^2} = c^2 \frac{\partial^2 \psi(t,x)}{\partial x^2}$$

provided that $\omega = \pm ck$. This is a special case, namely a non-dispersive wave propagation. Dispersive waves occur when ω is a function of k and the second derivative of ω is not identically zero. Here we have taken A as a constant, but generally, it does not need to be a constant, it can be time-dependent.

A wave packet is a linear combination of several plane waves, namely

$$\psi(t,x) = \sum_{k} B(t,k) e^{i(kx - \omega(k)t)}$$

where B(t, k) is the product of the coefficients of the linear combination and the amplitude of each plane wave.

A superposition may involve a continuously varying k over a given real interval or over all real axis. When this is the case, the sum in the wave packet becomes an integral over all real values of k. We have that B(t, k) becomes infinitesimal, namely B(t, k) = b(t, k)dk so that we have the following equation for the wave packet

$$\psi(t,k) = \int_{-\infty}^{\infty} b(t,k)e^{i(kx-\omega(k)t)}dk$$

The Fourier transform of $\psi(t, x)$ is given by

$$\hat{\psi}(t,k) = \sqrt{2\pi}b(t,k)e^{-i\omega(k)t}$$

Every function $\psi(t, x)$ that admits a Fourier transform can be considered as a wave packet.

Now that we know what a wave packet is, let us have a look at the following equation, which is the wave equation

~

$$(\partial_t^2 - \Delta_x)u = 0$$
$$u(0, x) = f(x)$$
$$\partial_t u(0, x) = g(x)$$

We can take the Fourier transform of this wave equation where we use the properties of Fourier transforms of derivatives that are discussed in part 3, which gives

$$(\partial_t^2 - i^2 |\xi|^2)\hat{u} = 0$$

By taking the Fourier transform of the wave equation, we obtain an equation that is easier to work with as we can factorize it into the following

$$(\partial_t - i|\xi|)(\partial_t + i|\xi|)\hat{u} = 0$$

which gives us $\partial_t \hat{u} = i |\xi| \hat{u}$ and $\partial_t \hat{u} = -i |\xi| \hat{u}$. These are both ordinary differential equations that we can solve. The solutions are given by

$$\hat{u}(t,\xi) = e^{\pm i|\xi|t+C}$$

where C is a constant. We see that we obtain two solutions which we need to match up to the initial conditions. this we also need to take the Fourier transforms of the initial conditions of the wave equation, which gives us

$$\hat{u}(0,\xi) = f(\xi)$$
$$\partial_t \hat{u}(0,\xi) = i\xi \hat{g}(\xi)$$

Using this first initial condition we find

$$\hat{u}(t,\xi) = e^{\pm i|\xi|t} \hat{f}(\xi)$$

From equations (2.100) (2.101) in [2] we obtain the following as we are also working in a spherical space

$$\hat{u}(t,\xi) = \frac{e^{\pm i|\xi|t}}{|\xi|}\hat{f}(\xi)$$

To find the solution to the wave equation we use our solutions to the ordinary differential equations to see that we obtain the following using the inverse Fourier transform

$$u(t,x) = \int_{-\infty}^{\infty} \frac{e^{\pm i|\xi|t}}{|\xi|} \hat{f}(\xi) e^{i|\xi|x} d\xi$$

As an example of an initial condition to the wave equation, we can take

$$f(x) = \sum c_n e^{\frac{-|x-x_n|^2}{\sigma}}$$

Taking the Fourier transform of f(x) and using the properties of the Gaussian integral we obtain

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} \sum c_n e^{\frac{-|x-x_n|^2}{\sigma}} e^{-i|\xi|x} dx$$
$$= \sum c_n \int_{-\infty}^{\infty} e^{\frac{-|x-x_n|^2}{\sigma} - i|\xi|x} dx$$
$$= \sum c_n \int_{-\infty}^{\infty} e^{-\frac{x^2}{\sigma} + (\frac{2x_n}{\sigma} - i|\xi|)x - \frac{x_n^2}{\sigma}} dx$$
$$= \sum c_n \sqrt{\pi\sigma} e^{\frac{x_n^2}{\sigma} - x_n i|\xi| - \frac{\sigma|\xi|^2}{4} - \frac{x_n^2}{\sigma}}$$
$$= \sum c_n \sqrt{\pi\sigma} e^{-\frac{\sigma|\xi|^2}{4}} e^{-x_n i|\xi|}$$

Now we have the initial condition that is needed to obtain the solution to the wave equation. The solution of the wave equation is now given by

$$u(t,x) = \int_{-\infty}^{\infty} \frac{e^{\pm i|\xi|t}}{|\xi|} \sum c_n \sqrt{\pi\sigma} e^{-\frac{\sigma|\xi|^2}{4}} e^{-x_n i|\xi|} e^{i|\xi|x} d\xi$$

This gives a nice tractable solution for generic Gaussian initial conditions.

7 What is an observability inequality

We have mentioned the Schrödinger equation before, we will now look at the observability for this equation. We take a look at the introduction of [7] where they define an observability inequality in the following way. An observation inequality for the Schrödinger equation is an inequality of the form

$$||\psi_0||^2_{L^2(\mathbb{R}^d)} \le C \int_0^T \int_\Omega |\psi(t,x)|^2 dx dt$$

for some T > 0, where Ω is an open subset of \mathbb{R}^d , and C is a positive constant, which holds for some appropriate class of initial data ψ_0 .

For the problem we want to study later on, we want to be more specific to our equation. For this reason, we look at how the observability equation is defined in [15] and give a short summary of the introduction of this paper. We take D, D_0 as bounded smooth subdomains of \mathbb{R}^d with $D_0 \subset D$. The equation that we consider is the controlled linear Schrödinger equation

$$\begin{split} i\partial_t u(t,x) &= -\Delta u(t,x) + V(t,x) u(t,x) + f(t,x) \mathbf{1}_{D_0}(x) & \text{in } (0,T) \times D \\ u(t,x) &= 0 & \text{on } (0,T) \times \partial D \\ u_0(x) &= u(0,x) & \text{in } D \end{split}$$

here u(t, x) is the state, f(t, x) is the control and V(t, x) is the potential, each of these can be a complex function. This system is well-posed in $L^2(D)$ with controls in $L^2((0,T) \times D)$ for $L^{\infty}((0,T) \times D)$ potentials [21].

The solution to the controlled linear Schrödinger equation with an L^{∞} potential is controllable to another state $u_T = u(T, x)$ if, provided the Hamiltonian flow, and the observation set satisfies the Geometric Control Condition. If a solution is observable, then often by duality the solution to the adjoint equation is controllable. Interior observability amounts to the solution u satisfying an estimate of the form

$$||u_0||_{L^2(D)} \le C_T ||u||_{L^2((0,T) \times D_0)}$$

for some nonzero C_T , $0 < T < \infty$.

Much is known about the observability problem for Schrödinger equations on a bounded domain with L^{∞} potentials. When we replace D with \mathbb{R}^d and D_0 , the support of the control, with $\omega = \mathbb{R}^d \setminus \overline{\Omega}$ where Ω is a bounded domain, much less is known about the observability problem for the Schrödinger equation. We now want to establish observability for

$$i\partial_t u = (-\kappa_1(t)\Delta + \kappa_2(t)|x|^2)u \quad 0 < t \le T, \quad x \in \mathbb{R}^d$$
$$u(0,x) = u_0(x)$$

where $\kappa_1(t) \in C^1([0,T])$, $\kappa_2 \in C([0,T])$ and u(0,x) is real valued and in a weighted $L^2(\mathbb{R}^d)$ space. This means that we want to establish a bound for the solution of the above partial differential equation as

$$||u_0||_{L^2(\mathbb{R}^d)} \le C_T ||u||_{L^2((0,T)\times\omega)}$$

which is challenging as ω is no longer bounded. The potential is not compactly supported, which makes the problem more challenging. The Schrödinger operator in the free space with a non-compactly supported potential behaves much differently.

Any quantum mechanical system with a potential energy V(x) has local equilibrium points which can be analysed by the model for a quadratic Hamiltonian,

where $\kappa_1(t) = \kappa_2(t) = \frac{1}{2}$. Taking the Taylor expansion of V(x) around the point x_0 gives

$$V(x) \approx V(x_0) + \nabla V(x_0)(x - x_0) + \frac{1}{2} \nabla^2 V(x_0)(x - x_0)^2$$

The second term of the expansion vanishes when x_0 is a critical point. We can translate x_0 to zero to obtain

$$V(x) \approx V(x_0) + \frac{1}{2}\nabla^2 V(x_0)x^2$$

this model is now reduced to the one of the harmonic oscillator. The Hamiltonian associated to this operator is $\frac{1}{2}(|p|^2 + |x|^2)$. The Hamiltonian ray path for this operator is computed by solving the system of ODEs

$$\frac{dx(t)}{dt} = p(t) \qquad \frac{dp(t)}{dt} = -x(t)$$

This operator has a cusp at zero, which means that there is one point for which the Hamiltonian ray path is such that $\frac{dx(t)}{dt} = 0$ which can affect the validity of a Gaussian wavepacket construction.

8 Main result

In this section we want to find u(t, x) that solves the following equation

$$i\partial_t u = \kappa_2(t)|x|^2 u + \Delta u$$

which is the equation with the time-quadratic operator where we take $\kappa_1(t) = 1$ and we have $0 \leq \kappa_2(t)$ depending continuously on time t for $0 \leq t \leq T$. Furthermore, we want to find the observability constant and the observation set for certain cases. Finding the observability constant is possible when the initial data is of a certain form.

We can look at the following example where we take the following initial conditions to this equation

$$f(x) = \frac{d^k}{dx^k} (e^{-x^2})$$

We have that the Fourier transform of this initial data is

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} \frac{d^k}{dx^k} (e^{-x^2}) e^{-i\xi x} dx$$
$$= (i\xi)^k \int_{-\infty}^{\infty} e^{-x^2} e^{-i\xi x} dx$$
$$= (i\xi)^k \sqrt{\pi} e^{-\frac{|\xi|^2}{4}}$$

where we use the Gaussian integral.

To be able to solve this equation we need the following lemma, which gives us the solution of the equation using the Fourier integral operator.

Lemma 8.1. Assume the Hamiltonian flow is non-zero for all $0 \le t \le T$. The associated FIO solution to

$$\frac{\partial}{\partial t}u(t,x) + iLu(t,x) = 0, \quad 0 < t \le T, \quad x \in \mathbb{R}^d$$

can be written as

$$u(t,x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{i\phi(t,x,\eta)} (a(t))^d \hat{u_0}(\eta) d\eta$$

The equality is understood for non- L^1 u_0 functions in the sense of distributions as above. The phase is of the form

$$i\phi(t, x, \eta) = iy_1(t)|x|^2 + iy_2(t)x \cdot \eta + iy_3(t)|\eta|^2$$

where $y_1(t), y_2(t), y_3(t)$ are functions of t as determined by the following system of ordinary differential equations

$$y'_{1}(t) = -4\kappa_{1}(t)(y_{1}(t))^{2} - \kappa_{2}(t) \qquad \qquad y_{1}(0) = 0$$

$$y'_{2}(t) = -4\kappa_{1}(t)y_{1}(t)y_{2}(t) \qquad \qquad y_{2}(0) = 1$$

$$y'_{3}(t) = -\kappa_{1}(t)y_{2}^{2}(t) \qquad \qquad y_{3}(0) = 0$$

and the amplitude satisfies

$$a(t) = e^{-2\int_0^t y_1(s)\kappa_1(s)ds}$$

The proof of this lemma can be found in [15]. An idea of this proof is given below. We have that the phase is given by $\phi(t, x, \eta) = y_1(t)|x|^2 + y_2(t)x \cdot \eta + y_3(t)|\eta|^2$. This phase must solve the eikonal equation $\frac{\partial}{\partial t}\phi + \kappa_1(t)|\nabla_x\phi|^2 + \kappa_2(t)|x|^2 = 0$. This gives us the following equation

$$y_1'(t)|x|^2 + y_2'(t)x \cdot \eta + y_3'(t)|\eta|^2 + 4y_1^2(t)|x|^2 + y_2^2(t)|\eta|^2 + 4y_1(t)y_2(t)x \cdot \eta + \kappa_2(t)|x|^2 = 0$$

We can now see that we get the system of ordinary differential equations.

To solve the equation we take this lemma with $\kappa_1 = 1$ and $\kappa_2 = \kappa_2$. Using the results from the lemma and $\hat{u}_0(\eta) = \hat{f}(\eta)$ we get

$$u(t,x) = \frac{a(t)}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{iy_1(t)|x|^2 + iy_2(t)x \cdot \eta + iy_3(t)|\eta|^2} (i\eta)^k \sqrt{\pi} e^{-\frac{|\eta|^2}{4}} d\eta$$

where $a(t) = e^{-2 \int_0^t y_1(s)}$. When we take k = 1 we obtain the following

$$u(t,x) = \frac{a(t)}{\sqrt{2}} \int_{-\infty}^{\infty} i\eta e^{iy_1(t)|x|^2 + iy_2(t)x \cdot \eta + (iy_3(t) - \frac{1}{4})|\eta|^2} d\eta$$
$$= \frac{-a(t)\sqrt{2\pi}2xy_2(t)e^{ix^2(y_1(t) - \frac{y_2^2(t)}{i + 4y_3(t)})}}{(1 - 4iy_3(t))^{\frac{3}{2}}}$$

Taking k = 2 gives

$$u(t,x) = \frac{a(t)}{\sqrt{2}} \int_{-\infty}^{\infty} (i\eta)^2 e^{iy_1(t)|x|^2 + iy_2(t)x \cdot \eta + (iy_3(t) - \frac{1}{4})|\eta|^2} d\eta$$
$$= \frac{a(t)\sqrt{2\pi}(4x^2y_2^2(t) + 8iy_3(t) - 2)e^{ix^2(y_1(t) - \frac{y_2^2(t)}{i + 4y_3(t)})}}{(1 - 4iy_3(t))^{\frac{5}{2}}}$$

Looking at these specific cases, we start to see a pattern. We recognize that the Hermite polynomials are in these equations.

We can find a generalized solution u(t, x) when we look at the pattern we observe from these different cases. Namely,

$$u(t,x) = \frac{(-1)^k a(t) \sqrt{2\pi} H_k(xy_2(t)) e^{ix^2(y_1(t) - \frac{y_2^2(t)}{i + 4y_3(t)})}}{(1 - 4iy_3(t))^{\frac{2k+1}{2}}}$$

To find the observability constant we take $u(t, x) = \phi_k(t, x)$.

We will have a look at the problem when we take time t = 0. This means that we have $y_1(0) = 0$, $y_2(0) = 1$ and $y_3(0) = 0$ and we also have $a(0) = e^{-2\int_0^0 y_1(s)ds} = 1$ by the lemma. Furthermore, at time t = 0, the Gaussians are normalized to be a constant. Substituting our findings into the function for ϕ we found before, we obtain the following

$$\phi_k(0,x) = \sqrt{2\pi} H_k(x) e^{-x^2}$$

The Gaussian normalization constant is now calculated by

$$\int_{-\infty}^{\infty} |Ae^{-x^2}|^2 dx = \sqrt{\frac{\pi}{2}}$$

This means that $A^2 = \sqrt{\frac{2}{\pi}}$ and thus the normalization constant is $A = \left(\frac{2}{\pi}\right)^{\frac{1}{4}}$.

Now we can take the inner products $\langle \phi_k, \phi_j \rangle$ where $k \neq j$ and $\langle \phi_k, \phi_k \rangle$, where we take time t = 0. To find the observability constant, we remove the plane below x = -10, so we get the following integrals.

$$\begin{split} \langle \phi_1, \phi_1 \rangle &= \int_{-10}^{\infty} (-\sqrt{2\pi} 2x e^{-x^2}) (-\sqrt{2\pi} 2x e^{-x^2}) e^{-x^2} dx \\ &= \frac{2}{9} \pi \left(-\frac{400}{e^{300}} + \sqrt{3\pi} (1 + \operatorname{erf}(10\sqrt{3})) \right) \\ \langle \phi_1, \phi_2 \rangle &= \int_{-10}^{\infty} (-\sqrt{2\pi} 2x e^{-x^2}) (\sqrt{2\pi} (4x^2 - 2) e^{-x^2}) e^{-x^2} dx \\ &= -\frac{2396\pi}{e^{300}} \\ \langle \phi_2, \phi_2 \rangle &= \int_{-10}^{\infty} (\sqrt{2\pi} (4x^2 - 2) e^{-x^2}) (\sqrt{2\pi} (4x^2 - 2) e^{-x^2}) e^{-x^2} dx \\ &= \frac{8}{9} \pi \left(-\frac{5970}{e^{300}} + \sqrt{3\pi} (1 + \operatorname{erf}(10\sqrt{3})) \right) \end{split}$$

Now with this, we can find the observability constant by taking the sum of these solutions to the inner products and dividing them by the sum of the normalization constants. This results in the following observability constant. This means that the observability constant is given by

$$\frac{\frac{2}{9}\pi \left(-\frac{400}{e^{300}} + \sqrt{3\pi}(1 + \operatorname{erf}(10\sqrt{3}))\right) - \frac{2396\pi}{e^{3}00} + \frac{8}{9}\pi \left(-\frac{5970}{e^{300}} + \sqrt{3\pi}(1 + \operatorname{erf}(10\sqrt{3}))\right)}{3\left(\frac{2}{\pi}\right)^{\frac{1}{4}}} = \frac{-\frac{7716\pi}{e^{300}} + \frac{10}{9}\pi\sqrt{2\pi}\operatorname{erf}(10\sqrt{3}) + \frac{10}{9}\pi}{3\left(\frac{2}{\pi}\right)^{\frac{1}{4}}}$$

From this example, we see we can that the observability constant is computable with a weight, which is an exact constant.

9 Conclusion

What can be concluded from the results in the last section is that we can find exact solutions to the equations with time-dependent operators of any time with a quadratic potential. These solutions have not been constructed before in literature except for in the paper [15] by Alden Waters, on which this paper was based. We see that this solution is written in terms of the Hermite polynomials, which can be done when the initial data takes a specific form. Furthermore, we have shown that one can find the observability constant when we have initial data of the same form as for the exact solution. We have also seen that taking generic Gaussian initial conditions to the wave equation leads to a tractable solution, which is different from what is done in most literature.

9.1 Future work

As was mentioned, the solutions to equations with time-dependent operators of any time with a quadratic potential have not been constructed before in literature. There is therefore a lot more research that can be done in this part of the field. Taking different initial conditions can lead to a difference in results. For example, one can take initial data that consists of Hermite functions. Future work can also include computing the observability constant using propagated Hermite polynomials. Using these propagated Hermite polynomials, the constant is closely approximated for generic B-valued initial data. In the papers [6] and [14], one can find more examples that use Gaussian wave packets to find solutions to specific problems.

References

- George B. Arfken, Hans J. Weber, and Frank E. Harris. "Chapter 18 -More Special Functions". In: *Mathematical Methods for Physicists (Seventh Edition)*. Ed. by George B. Arfken, Hans J. Weber, and Frank E. Harris. Seventh Edition. Boston: Academic Press, 2013, pp. 871-933. ISBN: 978-0-12-384654-9. DOI: https://doi.org/10.1016/B978-0-12-384654-9 .00018-9. URL: https://www.sciencedirect.com/science/article/ pii/B9780123846549000189.
- [2] Antonio Barletta. "Fourier Transform and Wave Packets". In: Routes to Absolute Instability in Porous Media. Cham: Springer International Publishing, 2019, pp. 7–27. ISBN: 978-3-030-06194-4. DOI: 10.1007/978-3-030 -06194-4_2. URL: https://doi.org/10.1007/978-3-030-06194-4_2.
- F.A. Berezin and M. Shubin. *The Schrödinger Equation*. Mathematics and its Applications. Springer Netherlands, 2012. ISBN: 9789401131544. URL: https://books.google.nl/books?id=fajzCAAAQBAJ.
- [4] Joel Feldman. Using the Fourier Transform to solve PDEs. Online: accessed 4-January-2023. 2007. URL: https://personal.math.ubc.ca/~feldman/ m267/pdeft.pdfjoe;.
- [5] D.A. Fleisch. A Student's Guide to the Schrödinger Equation. Student's Guides. Cambridge University Press, 2020. ISBN: 9781108834735. URL: https: //books.google.nl/books?id=VljPDwAAQBAJ.
- [6] Heiko Gimperlein and Alden Waters. "A Deterministic Optimal Design Problem for the Heat Equation". In: SIAM Journal on Control and Optimization 55.1 (2017), pp. 51–69. DOI: 10.1137/15M1031084. eprint: https: //doi.org/10.1137/15M1031084. URL: https://doi.org/10.1137/ 15M1031084.
- [7] François Golse and Thierry Paul. Observability for the Schrödinger Equation: an Optimal Transport Approach. 2021. DOI: 10.48550/ARXIV.2102.05155. URL: https://arxiv.org/abs/2102.05155.
- [8] A. Grigis and J. Sjostrand. Microlocal Analysis for Differential Operators: An Introduction. London Mathematical Society Lecture Notes. Cambridge University Press, 2014. ISBN: 9781299748866. URL: https://books.google .nl/books?id=XB%5C_moAEACAAJ.
- P.J. Olver. Introduction to Partial Differential Equations. Undergraduate Texts in Mathematics. Springer International Publishing, 2013. ISBN: 9783319020990. URL: https://books.google.nl/books?id=aQ8JAgAAQBAJ.

- [10] Karel Pravda-Starov. "Generalized Mehler formula for time-dependent non-selfadjoint quadratic operators". In: *Mathematische Annalen* 372 (Dec. 2018).
 DOI: 10.1007/s00208-018-1667-y. URL: https://arxiv.org/abs/1703.02797.
- [11] Henk de Snoo and Alef Sterk. *Functional analysis: an introduction*. University of Groningen, 2020.
- [12] Terrence Tao. *The Schrödinger equation*. URL: https://www.math.ucla .edu/~tao/preprints/schrodinger.pdf.
- W. Van Assche. "Ordinary Special Functions". In: Encyclopedia of Mathematical Physics. Ed. by Jean-Pierre Françoise, Gregory L. Naber, and Tsou Sheung Tsun. Oxford: Academic Press, 2006, pp. 637-645. ISBN: 978-0-12-512666-3. DOI: https://doi.org/10.1016/B0-12-512666-2/00395-3. URL: https://www.sciencedirect.com/science/article/pii/B0125126662003953.
- [14] Alden Waters. "A Parametrix Construction for the Wave Equation with Low Regularity Coefficients Using a Frame of Gaussians". In: *Communications* in mathematical sciences 9.1 (2011), pp. 225–254. ISSN: 1539-6746. DOI: 10.4310/CMS.2011.v9.n1.a11.
- [15] Alden Waters. Observability for Schrödinger equations with quadratic Hamiltonians. 2020. DOI: 10.48550/ARXIV.2011.10777. URL: https://arxiv.org/abs/2011.10777.
- [16] Wikipedia contributors. Error function Wikipedia, The Free Encyclopedia. [Online; accessed 3-January-2023]. 2022. URL: https://en.wikipedia .org/w/index.php?title=Error_function&oldid=1126231754.
- [17] Wikipedia contributors. Fourier transform Wikipedia, The Free Encyclopedia. [Online; accessed 4-January-2023]. 2023. URL: https://en.wikipedia .org/w/index.php?title=Fourier_transform&oldid=1130929023.
- [18] Wikipedia contributors. Gaussian integral Wikipedia, The Free Encyclopedia. [Online; accessed 3-January-2023]. 2022. URL: https://en.wikipedia .org/w/index.php?title=Gaussian_integral&oldid=1130517625.
- [19] Wikipedia contributors. Hermite polynomials Wikipedia, The Free Encyclopedia. [Online; accessed 4-January-2023]. 2023. URL: https://en.wikipedia.org/w/index.php?title=Hermite_polynomials&oldid=1131048800.
- [20] Wikipedia contributors. Wave Wikipedia, The Free Encyclopedia. [Online; accessed 4-January-2023]. 2022. URL: https://en.wikipedia.org/w/ index.php?title=Wave&oldid=1128707718.

[21] Enrique Zuazua. "Remarks on the controllability of the Schrödinger equation". In: vol. 33. Dec. 2003, pp. 193–211. ISBN: 9780821833308. DOI: 10.1090/crmp/033/12.