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Numerical solutions to the time-dependent Schrödinger equation for a model problem



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Abstract

This project delves into solving the time-dependent Schrödinger equation while using the one-dimensional harmonic oscillator as a model to avoid complications that arise from relativistic multi-dimensional quantum systems.

Starting from the ground state of the unperturbed system, we introduce a time-dependency by growing a bump in the middle. The dynamics of the system is then followed as the bump grows and perhaps disappears again.

The numerical solutions of the system are found by applying the finite difference method using Python, and the well-known solutions of the one-dimensional harmonic oscillator are then used for comparison.

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1 Introduction

Quantum mechanics emerged as a revolutionary theory in the early 20th century, experimental evidence then suggested that atomic particles behaved in a different way than expected, fundamentally altering our understanding of the physical world.

It started with Max Planck's groundbreaking move in the early 20th-century, where he (to explain black body radiation) proposed a solution that energy could only be emitted or absorbed in discrete, quantized form, "quanta" [1]. Shortly after, Einstein's postulate (explaining the mechanics of photoelectric effect [2]) was strongly supporting Planck's work, that light itself consists of individual quantum particles, or what we today call photons. Moving on to Niels Bohr's model of the atom [3], which was proposing that electrons orbit the nucleus in quantized energy levels, and that any transition between them results in emission/absorption of "photons" with discrete energies.

Fast forward to the mid-1920s, all of these efforts were successfully put together to be the first step in the formation of quantum mechanics, by Erwin Schrödinger, Werner Heisenberg, Max Born, and others [4].

Quantum mechanics was a major break-through, especially Schrödinger equation, explaining how particles with wave-like nature behave. It plays a role analogous to Newton's second law, but instead of looking for the particle's position, it considers its wave function, where the absolute square of the latter gives the probability of finding the particle in a particular region of space at a particular instant of time.

Schrödinger equation is central to all applications of quantum mechanics, as well as in comprehending and advancing technologies across various fields. This applies everywhere, from material science, aiming to develop advanced materials such as superconductors [5], to chemistry for deeper insights into chemical bonds and reactions [6], and notably in the realm of atomic physics, where the behavior of electrons within atoms reigns dominates and plays a crucial role in understanding what is happening on the atomic level [4].

Hence, throughout the years, a lot of new technologies were developed to help understand the quantum world in a better way, one of the most important branches that came to life after the formation of quantum mechanics is laser physics [7], which as the name indicates, is a field that focuses on the study of lasers, devices that emits light through a process of optical amplification based on the stimulated emission of electromagnetic radiation. The underlying process of stimulated emission is intricately described by quantum mechanical principles. Consequently, a key aspect in this field involves solving Schrödinger equation to better understand the energy levels, transition rates, and coherence properties of the atomic and molecular systems, and in order to continue refining and improving new techniques, solving the equation in the most efficient way is essential.

Therefore, in this project, we aim to solve the time-dependent Schrödinger equation for the harmonic oscillator numerically by employing the Finite Difference Method [8], the results will be then compared to the theoretical values and conclusions will be drawn.

2 Theory

2.1 Time-dependent Schrödinger equation

Given some initial conditions, usually at $t = 0$, the particle's wave function at future time, $\psi(x, t)$, is obtained by solving Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \psi = \hat{H}\psi \quad (1)$$

Where \hat{H} is the Hamiltonian operator ¹, which in one-dimensions is:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) \quad (2)$$

2.2 Algebraic solution to the harmonic oscillator

We will start with a time-independent system, that of the harmonic oscillator. The harmonic oscillator model gives a good first approximation in the neighborhood of a local minimum, say $x = x_0$. The potential in one dimension can therefore be expanded in a Taylor series about the minimum:

$$V(x) = V(x_0) + V'(x_0)(x - x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 + \dots \quad (3)$$

Since $x = x_0$ is a minimum, we can set $V'(x_0) = 0$ and $k = V''(x_0)$:

$$V(x) - V(x_0) \approx \frac{1}{2}k(x - x_0)^2 \quad (4)$$

By rearranging (5) and setting it in (2), the Hamiltonian operator can be written as follows:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \quad (5)$$

Using the momentum operator $\hat{p} \equiv i\hbar d/dx$ and factoring the Hamiltonian gives the following form of the time-independent Schrödinger equation:

$$\frac{1}{2m} \left[\hat{p}^2 + (m\omega \hat{x})^2 \right] \psi = E\psi \quad (6)$$

To find the solutions, the following operators are introduced ²:

$$\hat{a}_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}} (\mp i\hat{p} + mw\hat{x}) \quad (7)$$

Multiplying the lowering operator with the rising operator (in this specific order since operators are not commutative):

$$\hat{a}_- \hat{a}_+ = \frac{1}{2\hbar m\omega} \left[\hat{p}^2 + (m\omega \hat{x})^2 - im\omega(\hat{x}\hat{p} - \hat{p}\hat{x}) \right] \quad (8)$$

¹The total energy, sum of kinetic and potential energy operators.

²Ladder operators: used to climb up and down in energy.

Note that the last term in the bracket is the commutator of \hat{x} and \hat{p} :

$$\hat{a}_-\hat{a}_+ = \frac{1}{2\hbar m\omega} \left[\hat{p}^2 + (m\omega\hat{x})^2 \right] - \frac{i}{2\hbar} [\hat{x}, \hat{p}] \quad (9)$$

The last term is nothing but the canonical commutation relation ³:

$$[\hat{x}, \hat{p}] = i\hbar \quad (10)$$

Putting all of this together, the Hamiltonian can be written as follows:

$$\hat{H} = \hbar\omega \left(\hat{a}_+\hat{a}_- + \frac{1}{2} \right) \quad (11)$$

And the Schrödinger equation in terms of \hat{a}_\pm takes the form

$$\hbar\omega \left(\hat{a}_\pm \hat{a}_\mp \pm \frac{1}{2} \right) \psi = E\psi \quad (12)$$

To find the ground state wave function and energy, we will use the fact that when the lowering operator operates on the ground state, we get zero:

$$\hat{a}_- \psi_0 = 0 \quad (13)$$

Using this in equation (7) gives a differential equation with the following solution (after normalization):

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \quad (14)$$

The ground state energy is obtained by setting this in equation (13) and solving for E :

$$E_0 = \frac{1}{2}\hbar\omega \quad (15)$$

The excited states can be found by applying the rising operator repeatedly

$$\boxed{\psi_n(x) = A_n (\hat{a}_+)^n \psi_0(x)} \quad (16)$$

Where A_n is the normalization constant. The energy of an arbitrary state:

$$\boxed{E_n = \left(n + \frac{1}{2} \right) \hbar\omega} \quad (17)$$

³David J. Griffiths. Introduction to quantum mechanics, (3rd edition): Cambridge University Press.

In future sections, reduced units will be used to make equations and calculations easier and more straightforward. This means that lengths will be measured in units of $\sqrt{\frac{\hbar\omega}{m}}$ and energies in units of $\hbar\omega$. Time will then be given in units of $1/\omega$. Consequently, the harmonic oscillator will be oscillating with the angular frequency 1.

This is one approach to solve the Schrödinger equation for the quantum harmonic oscillator, another is the analytical method that uses power series and Hermite polynomials⁴ to find the wave functions and corresponding eigenvalues.

Nevertheless, the method that will be explored in this project is completely different, as mentioned in the introduction, the Schrödinger equation will be solved numerically using Python (method discussed in detail later in 3.1) and the values will be compared to those found using the algebraic approach.

2.3 Time-propagation operator

Assume that the wave function at time t is known, $\psi(x, t)$. The time-propagation operator⁵ can be used to find the wave function at an arbitrary time:

$$\Psi(t + \Delta t) = e^{-\frac{i}{\hbar} \int_t^{t+\Delta t} H(t) dt} \Psi(t) \quad (18)$$

This can be approximated to first order⁶:

$$e^{-\frac{i}{\hbar} \int_t^{t+\Delta t} H(t) dt} \approx e^{-iH(t)\Delta t/\hbar} \quad (19)$$

Let $\{|i\rangle\}$ be a complete and finite set of eigenstates to the Hamiltonian at a specific time t with the eigenvalue equation:

$$\hat{H} |i\rangle = E_i |i\rangle \quad (20)$$

Then the Hamiltonian in the exponent can act on those eigenstates and the exponential term can be written as follows:

$$e^{-iH(t)\Delta t/\hbar} = \sum_i e^{-iE_i(t)\Delta t/\hbar} |i\rangle \langle i| \quad (21)$$

Eq. (21) will be used to study the dynamics of the harmonic oscillator with a bump that grows and shrinks in time.

⁴A sequence of orthogonal polynomials.

⁵i.e propagates the wave function forward in time.

⁶Assuming the Hamiltonian doesn't explicitly depend on time, or that its time dependence is negligible over the time interval.

3 Methods

Since the perturbed quantum harmonic oscillator system is not an analytically solvable problem, we will instead solve it numerically by using the Finite difference method.

3.1 Finite difference method, FDM

The finite difference method is a numerical tool used to approximate solutions to differential equations by approximating derivatives with finite differences. In the case of Schrödinger equation, the continuous spatial domain is discretized and therefore the differential equation is transformed into a set of linear equations, which can easily be solved numerically. This section describes the mathematical formulation of the finite difference method applied to the one-dimensional time-independent Schrödinger equation.

Recall equation (2), which with a time-independent potential is:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m\omega^2 \hat{x}^2 \quad (22)$$

Introducing the dimensionless quantity $z = x\sqrt{\frac{m\omega}{\hbar}}$ to factorize the Hamiltonian as:

$$\hat{H} = \frac{\hbar\omega}{2} \left(\frac{\partial^2}{\partial z^2} + z^2 \right) \quad (23)$$

Schrödinger equation can be written as follows:

$$\frac{1}{2} \left(\frac{\partial^2}{\partial z^2} + z^2 \right) \Psi = \frac{E}{\hbar\omega} \Psi \quad (24)$$

Now, the finite difference approximation is used to express the second derivative in terms of the function itself, it assumes that the function can be expanded in a Taylor series around the desired point.

Considering the function is defined at x (we transition back to the x variable for clarity), the value of the wave function can be estimated around it:

$$\begin{aligned} \Psi(x+h) &= \Psi(x) + h \frac{\partial\Psi(x)}{\partial x} + \frac{h^2}{2} \frac{\partial^2\Psi(x)}{\partial x^2} + \frac{h^3}{6} \frac{\partial^3\Psi(x)}{\partial x^3} + \dots \\ \Psi(x-h) &= \Psi(x) - h \frac{\partial\Psi(x)}{\partial x} + \frac{h^2}{2} \frac{\partial^2\Psi(x)}{\partial x^2} - \frac{h^3}{6} \frac{\partial^3\Psi(x)}{\partial x^3} + \dots \end{aligned} \quad (25)$$

Some rearranging gives the following expression of the second derivative:

$$\frac{\partial^2\Psi(x)}{\partial x^2} = \frac{1}{h^2} (\Psi(x-h) - 2\Psi(x) + \Psi(x+h)) + \mathcal{O}(h^2) \quad (26)$$

The 1D-Schrödinger equation now takes the form:

$$\frac{1}{2h^2} [\Psi(x-h) - 2\Psi(x) + \Psi(x+h)] + V\Psi = E\Psi \quad (27)$$

Scaling the potential and energy values by a factor of 2

$$\frac{1}{h^2} [\Psi(x - h) - 2\Psi(x) + \Psi(x + h)] + 2V\Psi = 2E\Psi \quad (28)$$

Note that by scaling the energy by a factor 2, the energy values will instead be given by:

$$E_n = 2n + 1 \quad (29)$$

Now the Hamiltonian is given the form of a tri-diagonal matrix with $-2/h^2$ along the main diagonal, and $1/h^2$ along the two diagonals around the main one

$$\hat{H} = \frac{1}{h^2} \begin{pmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & \ddots & \ddots & & \vdots \\ 0 & & & & 0 \\ \vdots & \ddots & \ddots & & 1 \\ 0 & \dots & 0 & 1 & -2 \end{pmatrix} \quad (30)$$

Assuming there is no kinetic energy in the system, the energy at each grid point, x , should be equal to the potential energy. Therefore, the matrix $V(x)$ is diagonal with the potential energy along the main diagonal:

$$V(x) = \begin{pmatrix} V(x_1) & 0 & \dots & \dots & 0 \\ 0 & V(x_2) & 0 & \dots & 0 \\ \vdots & 0 & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & 0 \\ 0 & 0 & \dots & \dots & V(x_n) \end{pmatrix} \quad (31)$$

Last step is to add the potential energy to the Hamiltonian matrix, diagonalize it and find its eigenvalues and eigenvectors/functions.

3.2 Perturbing the system

The quantum system is now perturbed by adding an additional potential term to the Hamiltonian, the system is then time propagated, the new Hamiltonian can then be written, as shown in 3.3:

$$\hat{H}(t) = \hat{H}_\omega(x) + V(x, t) \quad (32)$$

3.2.1 Symmetric Gaussian potential

To maintain simplicity at the beginning, consider the perturbation as a Gaussian-shaped bump introduced into the harmonic oscillator potential, and positioned at its midpoint. The general form of a Gaussian function is:

$$V(x) = C_1 e^{-C_2 x^2} \quad (33)$$

Where the values of C_1 and C_2 will be chosen in a way such that a particle at the lowest energy levels will have to tunnel through the bump in order to go from one side to the other. The figure below displays three graphs, each figure illustrates the first five eigenstates of the unperturbed quantum harmonic oscillator. The symmetric Gaussian perturbation is added with different values of the constants.

In the first graph, we start with a moderate Gaussian perturbation by setting ($C_1 = C_2 = 1$), this slightly shifts the first few energy levels and eigenfunctions. The second graph shows a higher amplitude perturbation, resulting in more pronounced changes in the energy eigenvalues and wave functions. Lastly, the third graph illustrates the combined effect of a high amplitude and narrower width perturbation, causing a more significant deformation. These graphs highlights the varying impact of different Gaussian perturbations on the quantum harmonic oscillator.

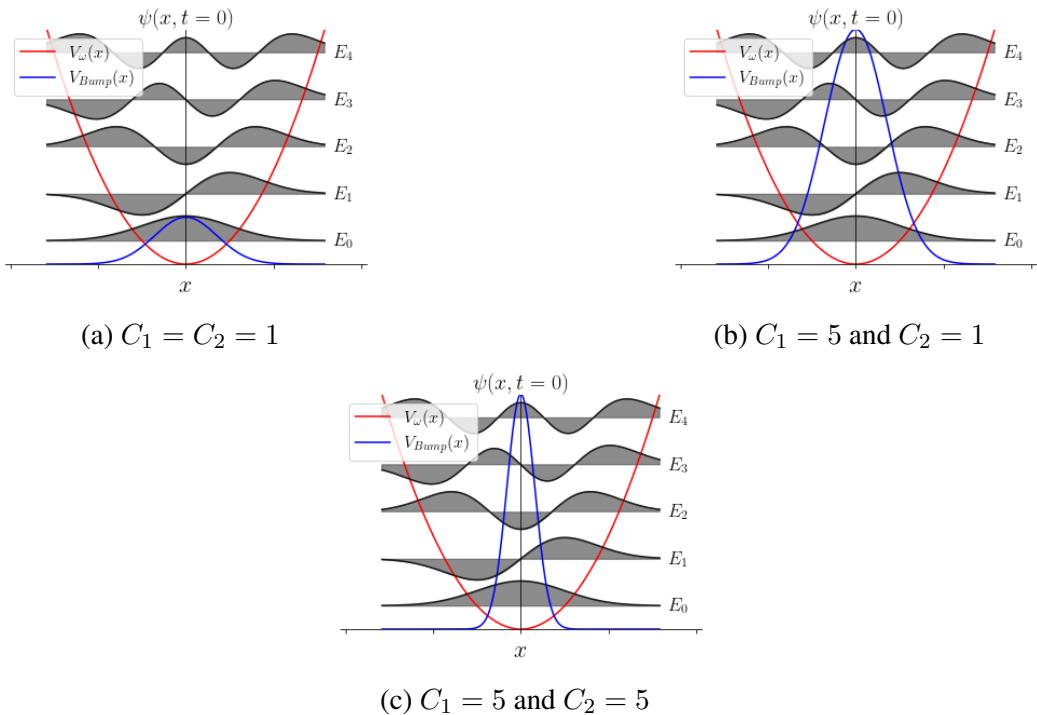


Figure 1: The Gaussian potential for different values of C_1 and C_2 .

As shown above, C_1 is the point at where the function intersects the y -axis while C_2 controls the width of it. It is worth to note that there is no optimal choice of those parameters, as long as they serve the case and affect the first wave functions as planned.

In future sections, the constants will take the following values:

$$C_1 = 10 \quad \text{and} \quad C_2 = 5 \quad (34)$$

3.2.2 Anti-symmetric bimodal Gaussian potential

To introduce a new perspective, we take a different route with a bit more complicated potential, namely an anti-symmetric Bimodal Gaussian function ⁷. When adding such potential to the typically symmetric quantum harmonic potential, the solutions to Schrödinger equation, which are typically either symmetric (even) or anti-symmetric (odd), will undergo mixing. This occurs because the anti-symmetric bimodal Gaussian potential breaks the original symmetry of the system. Consequently, the eigenfunctions are no longer purely even or odd, but rather a linear combination of both. this will lead to a more complex interaction between the potential and the system's wave functions.

The general form of a bimodal Gaussian potential:

$$V(x) = A_1 e^{-B_1(x-\mu_1)^2} - A_2 e^{-B_2(x-\mu_2)^2} \quad (35)$$

Where the constants, as mentioned in previous section, controls the appearance of the potential. In this case, A and B serves the same function as before, while μ represents the center of the peak. An anti-symmetric function has to fulfill:

$$V(-x) = -V(x) \quad (36)$$

Therefore, A_1 and A_2 should be equal

$$A_1 = A_2 \quad (37)$$

Similarly

$$B_1 = B_2 \quad (38)$$

And to make sure we get two different peaks, μ_1 and μ_2 must have opposite signs

$$\mu_1 = -\mu_2 \quad (39)$$

The figure below displays the first five eigenstates of the quantum harmonic oscillator along with an anti-symmetric bimodal Gaussian perturbation. This perturbation significantly alters the energy levels and eigenfunctions due to its anti-symmetric nature, resulting in a mixture of even and odd states and more complex modifications compared to the previous symmetric perturbation.

⁷A function that consists of two Gaussian functions with corresponding peak, resulting in a function with two distinct peaks, in this case a minimum and a maximum.

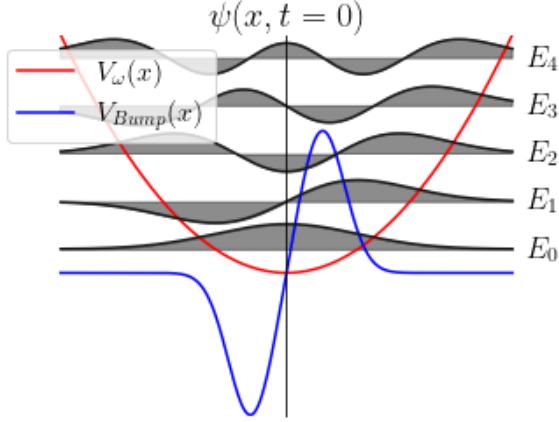


Figure 2: The Anti-symmetric Bimodal Gaussian potential.

In future sections, for simplicity, the constants will be assigned the following values:

$$A_1 = A_2 = B_1 = B_2 = 5 \quad \text{and} \quad \mu_1 = 0.5 \quad (40)$$

Now that the choice of the perturbation potentials is made, the next step involves allowing the system to evolve in time. This temporal propagation is crucial for capturing the dynamical behavior of the system under the influence of different perturbations.

3.3 Quantum dynamical harmonic oscillator

As shown in 2.2, the Hamiltonian of the harmonic oscillator is time-independent, let's denote it as $\hat{H}_\omega(x)$. When propagating the wave function in time, we get a dynamical system whose Hamiltonian is time-dependent

$$\hat{H}(t) = \hat{H}_\omega(x) + V(x, t) \quad (41)$$

The extra potential term is a result of perturbing the system and propagating it in time. By diagonalizing the Hamiltonian in every time-step and projecting the old solution on the eigenvectors to the new Hamiltonian, the wave function in a time t_{n+1} later can be found using equation (20) and (23):

$$\Psi(t_{n+1}) = \sum_i e^{-iE_i(t_{n+1})\Delta t/\hbar} |i_{n+1}\rangle \langle i_{n+1}| \Psi(t_n) \rangle \quad (42)$$

Where $E_i(t_{n+1})$ are the instantaneous eigenvalues and $|i_{n+1}\rangle$ are the eigenstates of the Hamiltonian, both at time t_{n+1} , and $\Delta t = t_{n+1} - t_n$ is a small time-step. The summation effectively propagates the wave function by taking into account the changes in the system's eigenstates and eigenvalues over each time-step.

Using a small time-step will give a more precise and detailed representation of the wave function's evolution over time. This method allows us to track how the system responds to the perturbations and evolves within the time-dependent potential, providing powerful insights into the dynamics of the quantum harmonic oscillator.

3.3.1 The energy of the system

In order to know how much energy the potential added to the system, we can find the average energy of the system by computing the expectation value of the Hamiltonian when the bump is over, and compare it to the initial eigenvalues of the unperturbed harmonic oscillator. At the end of the pulse, t_f , the wave function can be expressed as a sum of the eigenfunctions $|n\rangle$ corresponding to the unperturbed system:

$$\psi(t_f) = \sum_{n=0}^N c_n |n\rangle \quad (43)$$

The average energy in the state $|\psi(t)\rangle$ is given by:

$$\langle \hat{H}(t) \rangle = \langle \psi(t) | \hat{H}(t) | \psi(t) \rangle \quad (44)$$

We rewrite this expression in the state representation by inserting equation (44) in (45):

$$\langle \psi(t) | \hat{H}(t) | \psi(t) \rangle = \left(\sum_m c_m^* \langle m | \right) \hat{H}(t) \left(\sum_n c_n |n\rangle \right) \quad (45)$$

Since $|n\rangle$ are the eigenstates of \hat{H} , we know that

$$\hat{H} |n\rangle = E_n |n\rangle \quad (46)$$

Putting this together

$$\langle \psi(t) | \hat{H}(t) | \psi(t) \rangle = \sum_m \sum_n c_m^* c_n E_n \delta_{nm} \quad (47)$$

Using the orthonormality of the states the sum can be reduced to a single sum. We then get the following expression for average energy of the system:

$$\langle \hat{H}(t) \rangle = \sum_n |c_n|^2 E_n \quad (48)$$

4 Results

4.1 Unperturbed quantum harmonic oscillator

Before exploring the effects of perturbation, we will first show the solutions to the time-dependent Schrödinger equation for the unperturbed quantum harmonic oscillator using the finite difference method.

Figure 3 displays the harmonic oscillator potential along with first five eigenfunctions to the quantum harmonic oscillator at $t = 0$:

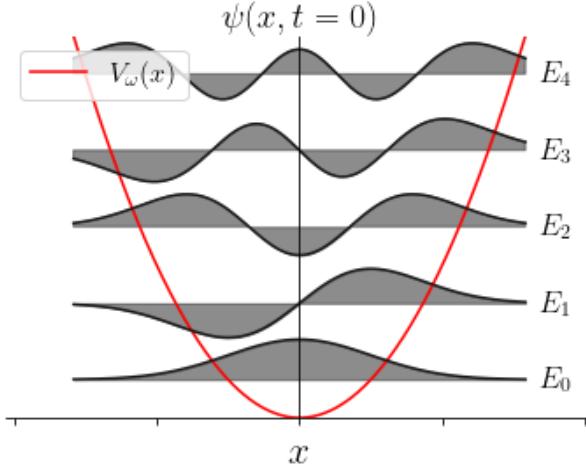


Figure 3: The first five eigenstates to the harmonic oscillator.

Following this graphical depiction. Table 1 presents the corresponding eigenvalues for those energy levels

n	$E_n/\hbar\omega$
0	1.00
1	3.00
2	5.00
3	7.00
4	9.00

Table 1: Energy values of the first 5 eigenstates for the unperturbed system.

It is worth of mention that the computed eigenvalues have been compared to the theoretical values obtained from analytical solutions, as shown in 2.2. The two approaches exhibit very good agreement, validating the accuracy of our numerical approach.

4.2 Perturbed quantum harmonic oscillator

4.2.1 Symmetric Gaussian potential

By establishing a reference point for comparison, we can now effectively evaluate the impact of the perturbations on the system's energy levels and wave functions.

For the symmetric Gaussian perturbation, the total potential acting on the system maintains its symmetry, as expected and shown below

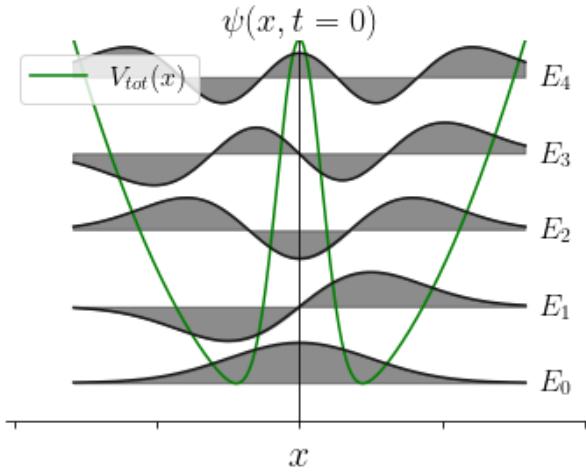


Figure 4: The total potential acting on the perturbed system.

Table 2 shows the energy of the first five states after perturbation

n	$E'_n/\hbar\omega$
0	3.18
1	3.49
2	6.87
3	7.60
4	10.41

Table 2: Energy values of the first 5 eigenstates after implementing the Symmetric bump.

This perturbation leads to noticeable alterations in the energy eigenvalues. It is worth to note that since the perturbation potential is symmetric around the origin, the symmetric states (corresponding to even quantum numbers $n = 0, 2, 4, \dots$) were the most affected. This observation is consistent with the properties of the wave functions. Similarly, the anti-symmetric states (corresponding to odd quantum numbers $n = 1, 3, 5, \dots$) are less susceptible to the symmetric perturbation since they have a node at the origin.

To further shed light on the impact of perturbation on the quantum harmonic oscillator,

figure 5 juxtaposes two sets of eigenfunctions side by side: the left figure shows the first five states of the unperturbed system, while the right figure shows the corresponding states after introducing the Gaussian perturbation.

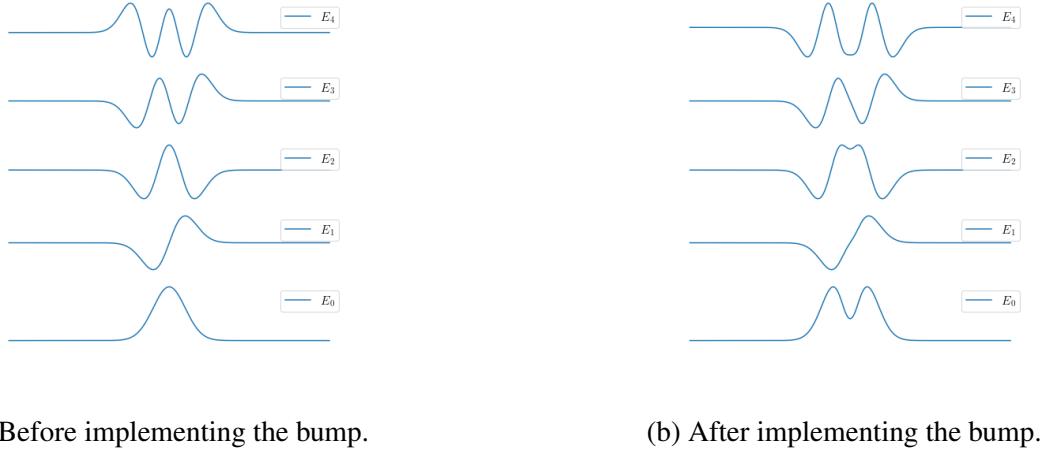


Figure 5: The first five eigenstates of the harmonic oscillator with an symmetric Gaussian potential perturbation.

4.2.2 Anti-symmetric bimodal Gaussian potential

Having established the baseline behavior of the perturbed quantum harmonic oscillator, we now move on to a slightly different perturbation, namely a bimodal anti-symmetric Gaussian potential. Figure 2 illustrates the total potential function acting on the system, resulting from the combination of the harmonic potential and the bimodal Gaussian potential

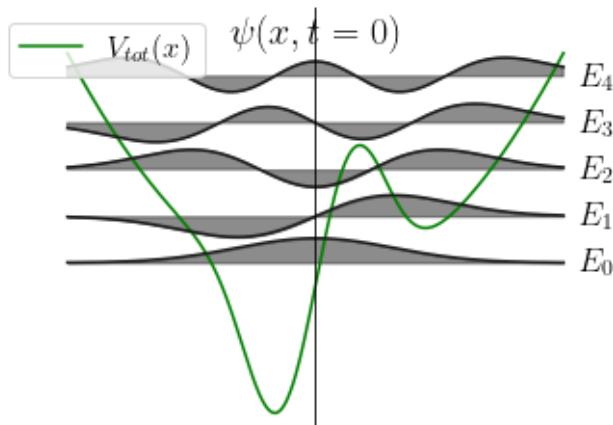


Figure 6: The total anti-symmetric potential acting on the perturbed system.

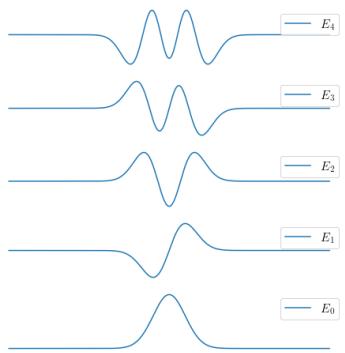
As mentioned earlier, the resulting potential is neither symmetric nor anti-symmetric, therefore, the behaviour of the wave functions is no longer following a symmetric/anti-symmetric pattern.

Table 3 shows the energy of the first 5 states after perturbation

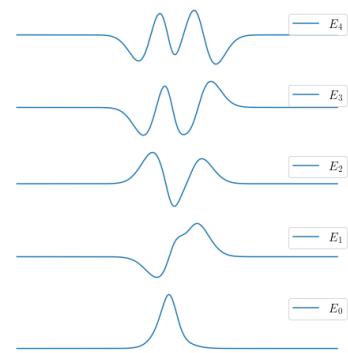
n	$E_n''/\hbar\omega$
0	0.24
1	3.35
2	5.09
3	7.05
4	9.03

Table 3: Energy values of the first 5 eigenstates after implementing the bump.

Similarly, figure 5 shows the first five eigenfunctions of the unperturbed and perturbed system side by side



(a) Before implementing the bump.



(b) After implementing the bump.

Figure 7: The first five eigenstates of the harmonic oscillator with an anti-symmetric Gaussian potential perturbation.

4.3 Sinusoidal Time-propagation

Now the system is left to propagate in time, as mentioned in 3.3, the Hamiltonian will take the form

$$\hat{H}(t) = \hat{H}_\omega(x) + V(x, t) \quad (49)$$

Since we are dealing with a harmonic oscillator which exhibits oscillatory behavior, a trigonometric function will be a good choice for the time-dependence term in order to capture the dynamics of the system in the best possible way (due to their periodic nature). The perturbation to the Hamiltonian takes the form

$$V(x, t) = V(x) \cdot V(t) \quad (50)$$

to make it straightforward, let $V(t)$ be the most simple trigonometric function

$$V(t) = \sin \Omega t, \quad 0 \leq t \leq \frac{\pi}{\Omega} \quad (51)$$

i.e $V(x, t)$ is only zero at the boundaries and non-zero between 0 and π/Ω .

The choice of Ω will determine the angular frequency of the perturbation, by setting $\Omega = \omega$, we ensure that the system oscillates with the same frequency as the unperturbed harmonic oscillator.

Now, by using the method mentioned in 3.3, we can find $\Psi(t_{n+1})$ in every time-step and plot it to get a clear animation of how the wave functions are propagated. The smaller the time-grids, the better we capture the dynamics of the system, for the sake of that, let

$$\Delta t = 0.01 \quad (52)$$

4.3.1 Symmetric Gaussian potential

For the symmetric Gaussian potential, the dynamics of the ground state are shown below, depicting the squared wave function (i.e., the probability) as a function of x

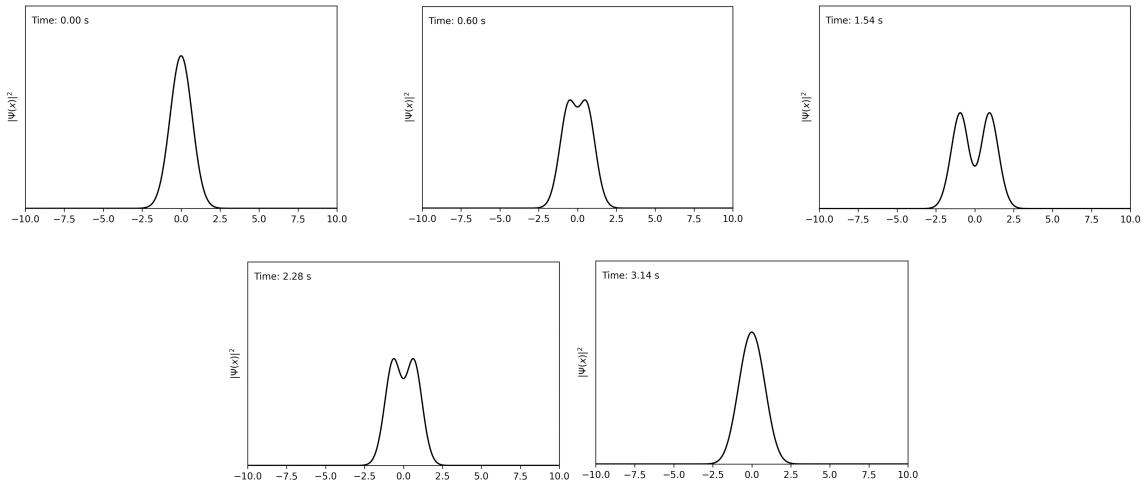


Figure 8: The ground state propagated under the influence of a symmetric perturbation over the interval $0 \leq t \leq \pi$.

As mentioned in 3.3.1, the wave function can be expressed as a sum of eigenfunctions corresponding to the unperturbed system at the end of the pulse. Therefore, equation (44) can be used to determine which eigenfunction dominates at the end, this entails calculating the constants c_n using their orthonormality property.

By taking the inner product of $\psi(t = \pi)$ with the respective $\langle n |$ from the left, we isolate the constant associated with each eigenfunction:

$$\langle n | \psi(t = \pi) \rangle = c_n \quad (53)$$

For each wave function $\psi(t = \pi)$, we determine the values of the constants by iterating n from 0 to N . Now we will let $N = 4$ for simplicity (Higher N have negligible contribution). This process enables us to anticipate the precise contribution of each eigenfunction to the resultant wave function at $t = \pi$.

For $\psi_0(t = \pi)$, the following values were obtained

$$\begin{cases} |c_0|^2 & \approx 0.982 \\ |c_1|^2 & \approx 0 \\ |c_2|^2 & \approx 0.018 \\ |c_3|^2 & \approx 0 \\ |c_4|^2 & \approx 0 \end{cases} \quad (54)$$

Where

$$\sum_{i=0}^4 |c_i|^2 \approx 1 \quad (55)$$

Since the harmonic oscillator and the perturbation are oscillating with the same angular frequency, at $t = \pi$, the wave function have done a whole cycle and gone back to its initial form, this is shown both in figure 8 and by the fact that $|c_0|^2$ is totally dominating over the other constants.

This phenomenon occurs because the potential energy within the system does not contribute to any net change in the total energy over one complete cycle.

Using equation (49), we get the following value for the average energy of the ground state at $t = \pi$:

$$\langle \hat{H} \rangle \approx 1.65 \quad (56)$$

Comparing this to the ground state energy of the unperturbed system, we see that there is no energy added to the system (taking the numerical uncertainties into account):

$$\langle \hat{H} \rangle - E_0 \approx 0 \quad (57)$$

By assigning a different angular frequency to the sine function compared to the unperturbed harmonic oscillator, net energy is introduced into the system. Consequently, the wave function does not return to its initial state at $t = \pi$ as shown below

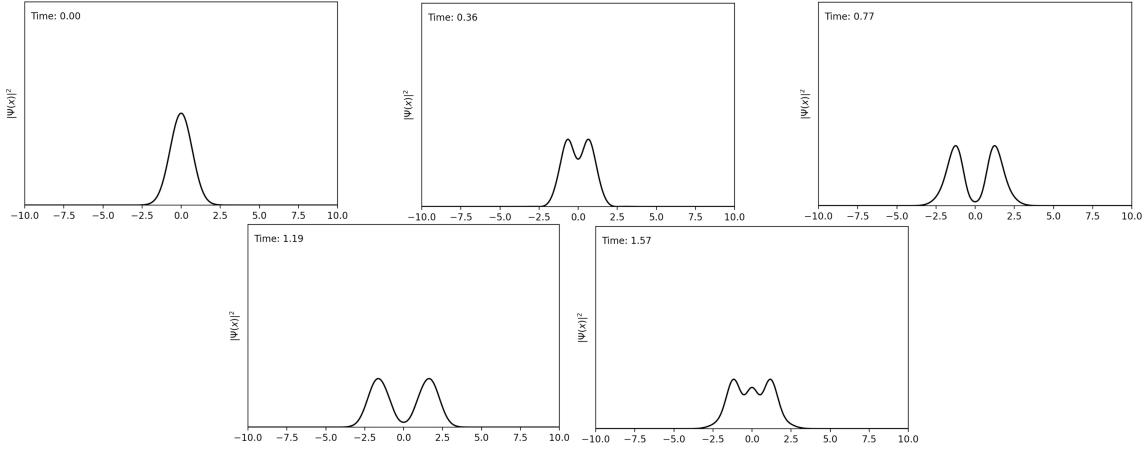


Figure 9: The ground state propagated with angular frequency 2ω under the influence of a symmetric perturbation over the interval $0 \leq t \leq \pi/2$.

Comparing the energies of the system before and after

$$\langle \hat{H} \rangle - E_0 \approx 2.31 > 0 \quad (58)$$

As seen in Table 2, the wave functions corresponding to odd quantum numbers n exhibit minimal impact from the perturbation compared to those with even quantum numbers. Therefore, the animations of the odd-numbered states are less notable and are therefore omitted here.

The dynamics of the second excited state are shown in the figure below.

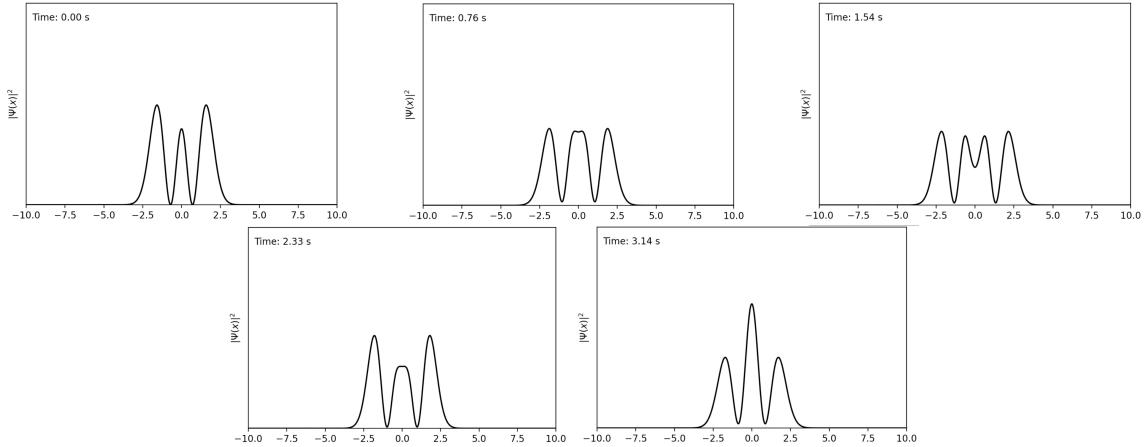


Figure 10: The second excited state propagated under the influence of a symmetric perturbation over the interval $0 \leq t \leq \pi$.

4.3.2 Anti-symmetric bimodal Gaussian potential

When the perturbation is anti-symmetric, it breaks the original symmetry and introduces asymmetry into the system, causing the wave functions to evolve in a more complex manner. The symmetry breaking leads to a more complex interaction between the wave functions and the potential, disrupting the simple periodic evolution observed in the symmetric case.

Due to the size and placement of the bump, the first two states are the most affected, as shown in Table 3.

The dynamics for the ground state is shown in the figure below

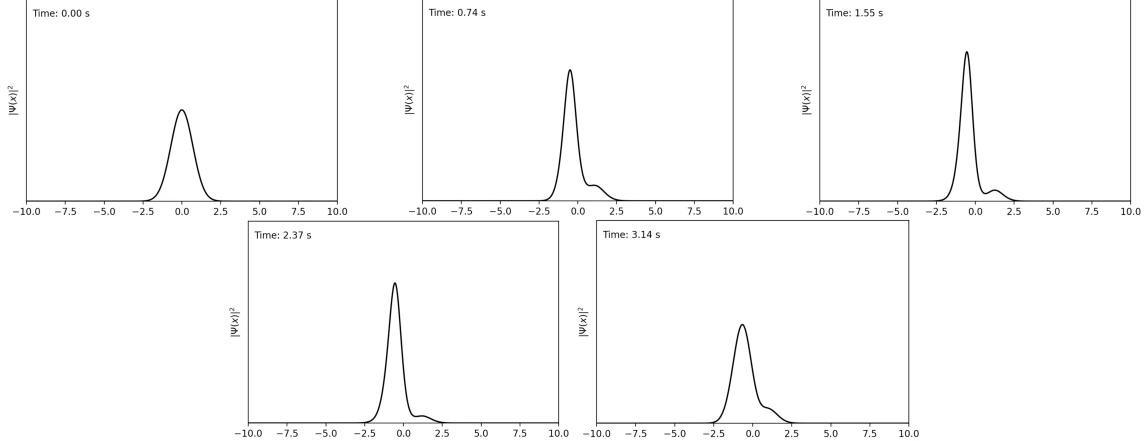


Figure 11: The ground state propagated under the influence of an anti-symmetric perturbation over the interval $0 \leq t \leq \pi$.

As seen in figure 11, the wave function does not return to its initial position, and hence the potential has added energy to the system, comparing it to the ground state energy we see that

$$\langle \hat{H} \rangle - E_0 \approx 0.83 > 0 \quad (59)$$

Similarly, the dynamics of the first excited state is shown below

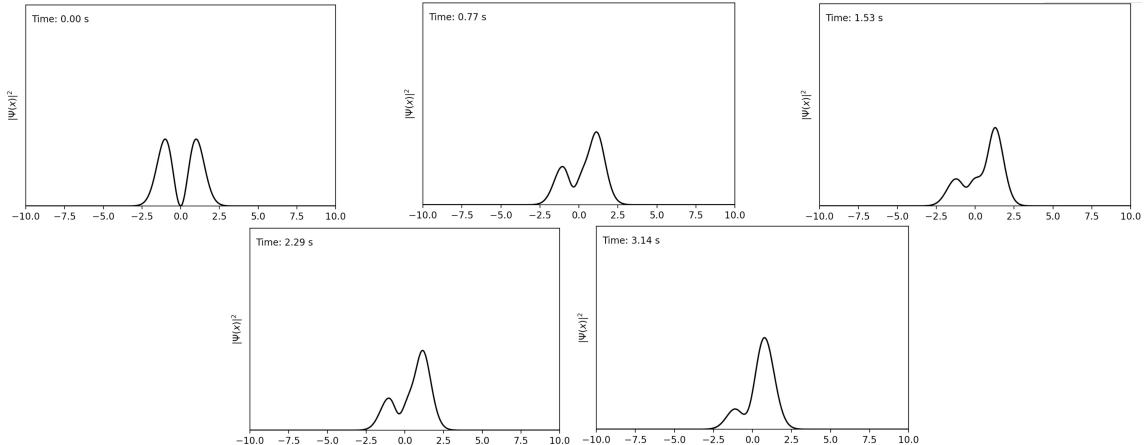


Figure 12: The first excited state propagated under the influence of an anti-symmetric perturbation over the interval $0 \leq t \leq \pi$.

These results demonstrate how the anti-symmetric perturbation significantly affects the system's dynamics. It causes a departure from the simple periodic behavior seen in the symmetric case, leading to a more complex evolution of the wave functions.

5 Discussion and conclusions

In this thesis, we aimed to solve the one-dimensional time-dependent Schrödinger equation for the quantum harmonic oscillator. The primary goal was to find the eigenvalues and eigenfunctions to the unperturbed system using the finite difference method, and then add a perturbation to explore and analyze how the system changes for different perturbation potentials. The finite difference method proved effective in solving Schrödinger equation by approximating the second derivative and diagonalizing the Hamiltonian matrix to find the eigenvalues and eigenfunction. The results obtained for the unperturbed system aligned perfectly with the well-known analytical solutions, validating the used numerical approach and allowing us to explore the system further.

Introducing perturbation to the system, namely a symmetric Gaussian potential and an anti-symmetric bimodal Gaussian potential, altered the eigenvalues and eigenfunctions of the system by different amounts. Due to the size and placement of the bump, the ground state of the system was the one effected the most.

The symmetric Gaussian potential shifted the energy levels of the system while maintaining the overall symmetry of the wave functions, while the anti-symmetric Gaussian potential also affected the overall symmetry of system, which highlights how quantum systems have different levels of sensitivity to different types of potentials, providing valuable insights into how to manipulate quantum systems. Lastly, we observed the evolution of the wave functions under the influence of a time-varying potential, which more accurately reflects real-world scenarios. The dynamics of the system were then captured and analyzed to better understand how quantum systems behave in reality.

To further improve the accuracy of this work, future studies could explore several potential improvements, one such involves the finite difference method itself. By using a five-point stencil for approximating derivatives instead of three, discretization errors could be reduced and the numerical accuracy of the solutions could be significantly increased, providing more precise solutions.

Other improvements includes investigating the effects of different time-dependent potentials, extending the study to higher-dimensional systems or incorporating more complex perturbations. This could further broaden our understanding of more complex quantum systems and their applications.

In summary, this approach in solving the one-dimensional time-dependent Schrödinger equation is big step forward in the world of quantum mechanics. It highlights the power of numerical methods in solving complex problems in a more time-efficient way, and how we can use this powerful tools to better model and visualize how different potentials impact quantum systems. It also paves the way for future studies to explore more complex systems and deepen our understanding of the quantum world.

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