

What electron feels under oscillating time-dependent perturbation in asymmetric double harmonic well

A SUMMER PROJECT REPORT

Submitted by

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1 Introduction

1.1 The Schrodinger equation

The state of any system is completely specified if its wavefunction (denoted by $\Psi(x, t)$) is known. Here $\Psi(x, t) \in \mathbb{C}$ generally. $|\Psi(x, t)|^2 dx$ gives the probability of finding the particle in the region dx at time t . If we know $\Psi(x, 0)$ for initial time ($t = 0$), we can determine $\Psi(x, t)$ for any time t by

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V(x, t) \Psi(x, t) \quad (1)$$

Equation(1) is called Time-dependent Schrodinger equation(TDSE). If the potential only depends on position i.e. $V(x, t) \equiv V(x)$ then we can attempt a separation of variables to the equation(1),

$$\Psi(x, t) = \psi(x)\phi(t) \quad (2)$$

Solving for (1) and (2) we obtain

$$\phi(t) = e^{-iEt/\hbar} \quad (3)$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x) \quad (4)$$

$\psi(x)$ obtained from equation(4) is called Time-independent Schrodinger equation(TISE). So the complete wavefunction of a system in potential $V(x)$ is

$$\Psi(x, t) = \psi(x)e^{-iEt/\hbar} \quad (5)$$

These states are called **stationary states** with energy E ($E \in \mathbb{R}$ and $E > V(x)_{min}$) as with time the probability distribution of the system does not change

$$|\Psi(x, t)|^2 = \psi(x)e^{-iEt/\hbar}\psi(x)^*e^{iEt/\hbar} = |\psi(x)|^2 \quad (6)$$

1.2 Harmonic Potentials

1.2.1 Harmonic well

The harmonic potential is defined by

$$V(x) = \frac{1}{2}kx^2 \quad (7)$$

1.2.2 Coupled-Harmonic well

We can now think of combining two harmonic systems to create the following system (which I call Coupled-harmonic well)

$$V(x) = -\frac{1}{2}\alpha x^2 + \frac{1}{4}\beta x^4 \quad (8)$$

Now we solve for minima by setting $V'(x) = 0$. So

$$\frac{\partial V(x)}{\partial x} = -\alpha x + \beta x^3 = 0 \quad (9)$$

solving for x we have :

$$x = 0 \quad or \quad x = \pm \sqrt{\frac{\alpha}{\beta}} \quad (10)$$

Now we look at $V(x)$ at these minima :

$$V\left(\pm \sqrt{\frac{\alpha}{\beta}}\right) = -\frac{1}{4}\frac{\alpha^2}{\beta} \quad (11)$$

Now let

$$\epsilon = \frac{1}{4}\frac{\alpha^2}{\beta} \quad and \quad a = \sqrt{\frac{\alpha}{\beta}} \quad (12)$$

Here a gives the distance of the two stable minima from origin and ϵ gives the depth of these from origin .Using (12) we can rewrite equation(8) as follows:

$$V(x) = -\frac{2\epsilon}{a^2}x^2 + \frac{\epsilon}{a^4}x^4 \quad (13)$$

1.2.3 Asymmetric Coupled-harmonic well

Till now both the terms in $V(x)$ were symmetric function of x . Now if we introduce an asymmetric function of x then our potential becomes asymmetric.

We introduce an x^3 term .

$$V(x) = -\frac{2\epsilon}{a^2}x^2 + \frac{\epsilon}{a^4}x^4 + \gamma x^3 \quad (14)$$

1.3 Superposition and time-evolution

Any $\Psi(x, 0)$ can be expressed as the superposition of the stationary states for a given potential.

$$\Psi(x, 0) = \sum_{i=0}^n c_n \psi_n(x) \quad (15)$$

We can now apply Fourier's trick to find c_n as follows:

$$c_n = \int \psi_n(x)^* \Psi(x, 0) dx \quad (16)$$

Once we know all c_n then $\Psi(x, 0)$ evolves in time as :

$$\Psi(x, t) = \sum_{i=0}^n c_n \psi_n(x) e^{-iE_n t/\hbar} \quad (17)$$

1.4 Perturbation theory

TISE is written in operator form as

$$\hat{H}\psi = E\psi \quad (18)$$

where \hat{H} is the Hamiltonian operator given by

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \quad (19)$$

We can easily solve the TISE for simple systems, but sometimes these simple systems can be little bit perturbed(disturbed). We can then use Perturbation theory to calculate the properties of the perturbed system. Based on the time dependence of the perturbation we have two class of theories .

1.4.1 Time-independent Perturbation theory

Our system can be either degenerate(many states correspond to same energy) or non-degenerate.

Non-degenerate case :

If the system is non-degenerate then the energy levels are either raised or lowered. Actual Hamiltonian of the system is

$$\hat{H} = \hat{H}^0 + \lambda \hat{H}' \quad (20)$$

where \hat{H}^0 is the initial Hamiltonian , \hat{H}' is the perturbation and λ is the extent of perturbation with $0 < \lambda < 1$.

We try to calculate the corrected energy and corrected wavefunctions by

$$\psi_n = \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots \quad (21)$$

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots \quad (22)$$

The superscripts represent the order of correction. Using equations (20), (21) and (22) in (18) we have:

$$(\hat{H}^0 + \lambda \hat{H}')[\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots] = (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots)[\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots] \quad (23)$$

The above is a power series expansion (assuming the corrections converge) in λ which allows us to compare the terms with same coefficients and compute the different correction terms. Like, the first order correction in energy is :

$$E_n^1 = \int \psi_n^{0*} \hat{H} \psi_n^0 dx \quad (24)$$

and the first-order correction in ψ_n is :

$$\psi_n^1 = \sum_{m \neq n} \frac{\int \psi_m^{0*} \hat{H} \psi_n^0 dx}{E_n^0 - E_m^0} \psi_m^0 \quad (25)$$

Degenerate case :

If our system was initially degenerate, then upon perturbation we will see the splitting of degenerate states.

Assuming our system to be two-fold degenerate i.e.

$$\hat{H}^0 \psi_a^0 = E^0 \psi_a^0 \quad \text{and} \quad \hat{H}^0 \psi_b^0 = E^0 \psi_b^0 \quad (26)$$

We can then show the energy gets split as follows:

$$E_{\pm}^1 = \frac{1}{2} \left[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2} \right] \quad (27)$$

where

$$W_{ij} = \int \psi_i^{0*} \hat{H} \psi_j^0 dx \quad (28)$$

Similarly we can show the splitting in n-fold degeneracy also.

1.4.2 Time-dependent Perturbation theory

When the disturbance depends on time, there is transition between one energy level to another. If we have just two levels in a system i.e.

$$\hat{H}^0\psi_a^0 = E^0\psi_a^0 \quad \text{and} \quad \hat{H}^0\psi_b^0 = E^0\psi_b^0 \quad (29)$$

We can now take the initial state to be the linear combination

$$\Psi(0) = c_a\psi_a + c_b\psi_b \quad (\text{such that } |c_a|^2 + |c_b|^2 = 1) \quad (30)$$

Now if we consider the perturbation $\hat{H}'(t)$ then $\Psi(t)$ can still be expressed as a linear combination but now the coefficients will depend on time as

$$\Psi(t) = c_a(t)\psi_a e^{-iE_a t/\hbar} + c_b(t)\psi_b e^{-iE_b t/\hbar} \quad (31)$$

Putting this in

$$\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad \text{where} \quad \hat{H} = \hat{H}^0 + \hat{H}'(t) \quad (32)$$

we can get

$$\frac{\partial c_a}{\partial t} = -\frac{i}{\hbar} \left[c_a H'_{aa} + c_b H'_{ab} e^{-i(E_b - E_a)t/\hbar} \right] \quad (33)$$

$$\frac{\partial c_b}{\partial t} = -\frac{i}{\hbar} \left[c_b H'_{bb} + c_a H'_{ba} e^{i(E_b - E_a)t/\hbar} \right] \quad (34)$$

where

$$H'_{ij} = \int \psi_i^{0*} \hat{H}' \psi_j^0 dx \quad (35)$$

Solving the above gives $c_a(t)$ and $c_b(t)$ which shows the coefficients itself changes with time (i.e. there is transition from one energy level to another of the system) due to time-dependent perturbation. Similarly we can show this for multi-level systems also.

1.5 Adiabatic approximation

The processes which are carried out very slowly such that the system remains almost unaffected, are referred to as **adiabtic processes**. So suppose a system is oscillating at its natural frequency ω_0 and now we are externally disturbing the system with frequency ω_{ext} .

If $\omega_{ext} \ll \omega_0$, the system is almost undisturbed and continues to oscillate with ω_0 . Otherwise if $\omega_{ext} \geq \omega_0$, the natural oscillations of the system gets affected. This is called **non-adiabatic process**.

Adiabatic Theorem in Quantum mechanics :

Let the Hamiltonian of the system changes from some initial form \hat{H}_i to final form \hat{H}_f . If the particle was initially in n^{th} eigenstate of \hat{H}_i , it will be carried (under schrodinger equation) into n^{th} eigenstate of \hat{H}_f i.e.

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = \hat{H} \Psi(t) = E_n(t) \Psi(t) \quad (36)$$

or in general if the system started with the state

$$\Psi = \sum_n c_n(t) \phi_n \quad (37)$$

Then this evolves according to

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = \hat{H} \Psi(t) \quad (38)$$

and at each instant

$$\hat{H} \Psi(t) \approx E_n(t) \Psi(t) \quad (39)$$

2 Methods

Most of the systems we deal with are complicated and cannot be solved analytically. So now we turn to solve our systems numerically for fairly approximate solutions. All the simulations to be done has been coded in Python-3.6.4. To test the correctness of codes, these has been tested on simpler systems(like the infinte well) for which the analytical solutions are already known.

2.1 Numerical solution of TISE

2.1.1 Numerov method

$$\frac{d^2y}{dx^2} = f(x)y + g(x) \quad (40)$$

Any ordinary-differential equation(ODE) of the above form ,which has a given initial condition(i.e. $y(x = x_0)$) can be solved numerically by Numerov's method which is

$$y_{m+1} = \frac{(12 - 10u_m)y_m - u_{m-1}y_{m-1}}{u_{m+1}} + \frac{1}{12} \frac{g_{m+1}10g_m + g_{m-1}}{u_{m+1}} h^2 + O(\Delta x^6) \quad (41)$$

with

$$u_m = 1 - \frac{1}{12} h^2 f_m \quad (42)$$

2.2 Shooting method for two point problems

Sometimes we have two unknowns(the function f itself and some constant= k) in our two-point ODE (where two boundary conditions $f(x_0)$ and $f(x_n)$ are known). We can solve these type of ODE's by shooting method. This is a

hit and trial method which simply is:

- 1) Choose some value of k (some reasonable value)
- 2) For this k solve the problem with initial condition $f(x_0)$
- 3) If $f(x_n)_{obtained} = f(x_n)_{given}$ then k is correct ,else search for a different k and repeat from step(1).

We have to devise a reasonable searching algorithm for different kind of problems provided.

2.3 Solving 1-D TISE numerically

2.3.1 Numerov method to TISE

We have equation(4) representing TISE for a single particle in 1-D. Setting $\hbar = 1$ and $m = 1$ (Hartree units) in equation(4) we get

$$-\frac{1}{2} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x) \quad (43)$$

Rearranging this gives

$$\frac{\partial^2 \psi(x)}{\partial x^2} = 2[V(x) - E]\psi(x) \quad (44)$$

Equation(44) is the same as equation(40) except here the $g(x)$ term is missing.

So we can apply equations (41) and (42) as follows:

$$\psi_{m+1} = \frac{(12 - 10u_m)\psi_m - u_{m-1}\psi_{m-1}}{u_{m+1}} \quad (45)$$

with

$$u_m = 1 - \frac{1}{6}h^2[V(x_m) - E] \quad (46)$$

2.3.2 Computing ψ and E by shooting method

We have our boundary conditions as $\psi(\pm\infty) = 0$. Now we apply shooting method to find ψ and E as follows:

1) Make a list of E values with reasonable spacing like

$$E_{possible} = [0, 0.1, 0.2, \dots]$$

2) Take first element of E_{list} as E .

3) Set an error bar, ϵ .

3) Compute $\psi(x = x_n)$ using $\psi(x = x_n) = 0$ in Numerov method. If $\psi(x_n) < \epsilon$, store this value in a list E_{list} and the ψ generated in another list ψ_{list} . This is one of the correct E and ψ . Move to step(1) with next value in $E_{possible}$.

4) If $\psi(x_n) > \epsilon$, look for the sign of $\psi(x_n)$ and compare with $\psi(x_n)$ of previous E -value.

4.1) if sign changes then use binary search for E values within these two until $\psi(x_n) < \epsilon$ and store these values. Repeat from step(1) using next value in $E_{possible}$.

4.2) else repeat from step(1) using next value in $E_{possible}$.

2.4 Solving 1-D TDSE numerically

2.4.1 Crank-Nicolson method for parabolic PDE's

$$\frac{\partial u(x, t)}{\partial t} = \alpha^2 \frac{\partial^2 u(x, t)}{\partial x^2} \quad (47)$$

Equations of the above form are called Parabolic- partial differential equations (PDE's). If an initial $u(x, t_0)$ is known, this can be solved numerically by a method developed by Crank and Nicolson. We have the time-derivative given

by forward-differences as :

$$\frac{\partial u_i^j}{\partial t} = \frac{u_i^{j+1} - u_i^j}{\Delta t} \quad (48)$$

and the position double-derivative according to Crank-Nicolson is taken as the average of the central differences at $t = j$ and $t = j + 1$ as follows:

$$\frac{\partial^2 u_i^j}{\partial x^2} = \frac{1}{2} \left[\frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\Delta x^2} + \frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{\Delta x^2} \right] \quad (49)$$

where

$$u_i^j = u(x = x_i, t = t_j) \quad (50)$$

The advantage of averaging is that when we put equation (48) and (49) in (47) , then we obtain the net error of order $O(\Delta t^2 + \Delta x^2)$.

2.4.2 Crank-Nicolson method on TDSE

We have the TDSE in 1-D given by equation(1). If we now set $\hbar = 1$ and $m = 1$ (Hartree units) then after rearrangement it looks like

$$\frac{\partial \Psi(x, t)}{\partial t} = \frac{i}{2} \frac{\partial^2 \Psi(x, t)}{\partial x^2} - iV(x, t)\Psi(x, t) \quad (51)$$

This is a Parabolic-PDE and applying Crank-Nicolson we get:

$$\frac{\partial \Psi_i^j}{\partial t} = \frac{\Psi_i^{j+1} - \Psi_i^j}{\Delta t} \quad (52)$$

$$\frac{\partial^2 \Psi_i^j}{\partial x^2} = \frac{1}{2} \left[\frac{\Psi_{i+1}^j - 2\Psi_i^j + \Psi_{i-1}^j}{\Delta x^2} + \frac{\Psi_{i+1}^{j+1} - 2\Psi_i^{j+1} + \Psi_{i-1}^{j+1}}{\Delta x^2} \right] \quad (53)$$

Putting equations(52) and (53) in (51) and rearranging we get:

$$-\lambda(\Psi_{i+1}^{j+1}\Psi_{i-1}^{j+1}) + (1 + 2\lambda + \frac{iV_i^{j+1}\Delta t}{2})\Psi_i^{j+1} = \lambda(\Psi_{i+1}^j\Psi_{i-1}^j) + (1 - 2\lambda - \frac{iV_i^j\Delta t}{2})\Psi_i^j \quad (54)$$

Here

$$\lambda = \frac{i\Delta t}{4\Delta x^2} \quad (55)$$

Equation(54) lets us create a recursion relation

$$A\Psi^{j+1} = B\Psi^j \quad (56)$$

where A and B are tri-diagonal matrices

$$A = \begin{pmatrix} A_1 & -\lambda & 0 & \dots & 0 \\ -\lambda & A_2 & -\lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -\lambda & A_{n-1} & -\lambda \\ 0 & \dots & 0 & -\lambda & A_n \end{pmatrix} \quad B = \begin{pmatrix} B_1 & \lambda & 0 & \dots & 0 \\ \lambda & B_2 & \lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \lambda & B_{n-1} & \lambda \\ 0 & \dots & 0 & \lambda & B_n \end{pmatrix}$$

where

$$A_i = 1 + 2\lambda + \frac{iV_i^{j+1}\Delta t}{2} \quad \text{and} \quad B_i = 1 - 2\lambda - \frac{iV_i^j\Delta t}{2} \quad (57)$$

If we know $\Psi(x, 0)$ then we can compute $\Psi(x, t)$ at ant later time t by (56).

3 Results and analysis

3.1 Eigenstates of harmonic and Coupled-harmonic well

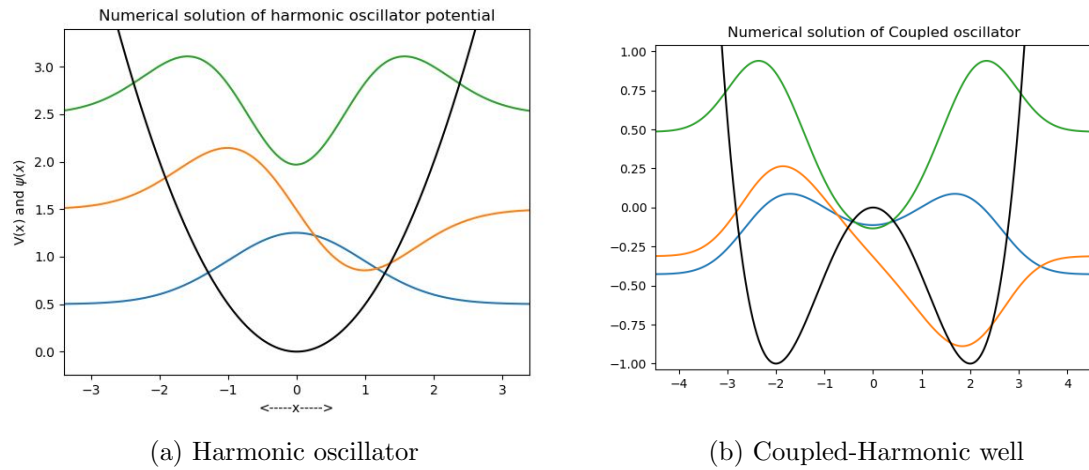


Figure 1: First three eigenstates arranged according to energy levels

3.2 Closer look at lower states

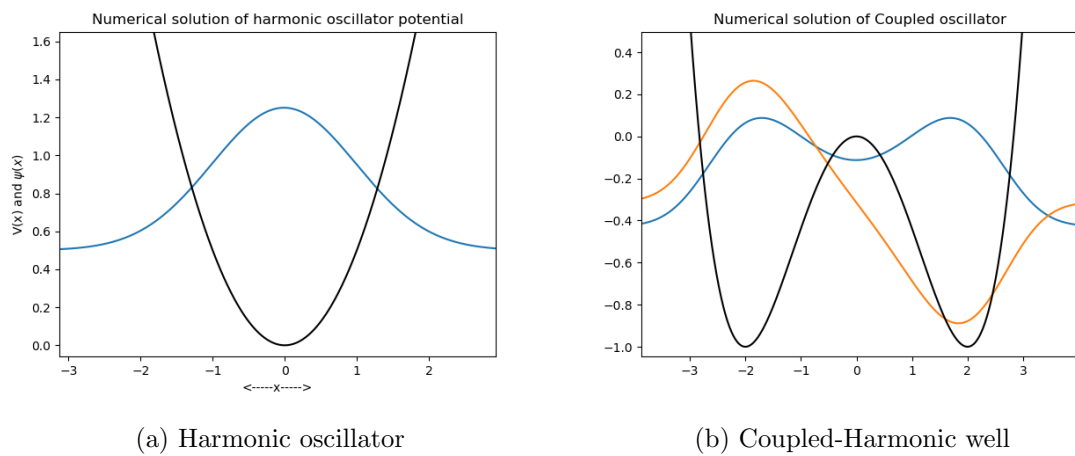


Figure 2: Comparison of ground-state eigenstates

If we look at the first two eigensates of the coupled well then we can clearly see the splitting of the two states(one of them is slightly raised in energy). This can be explained as follows:

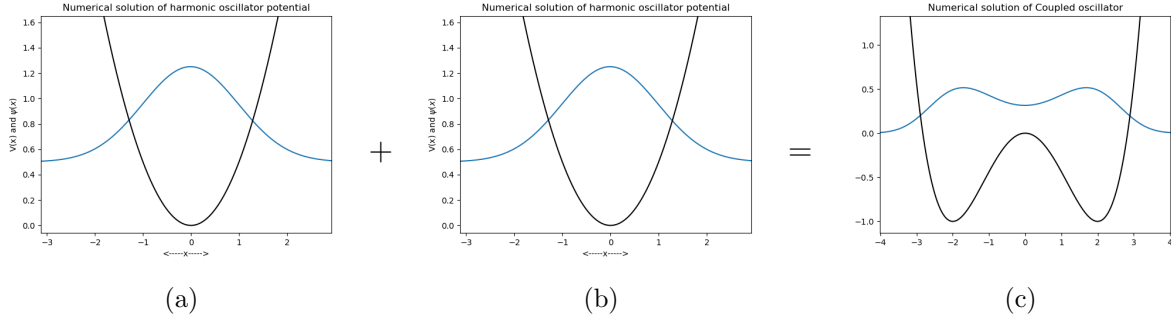


Figure 3: Constructive overlap

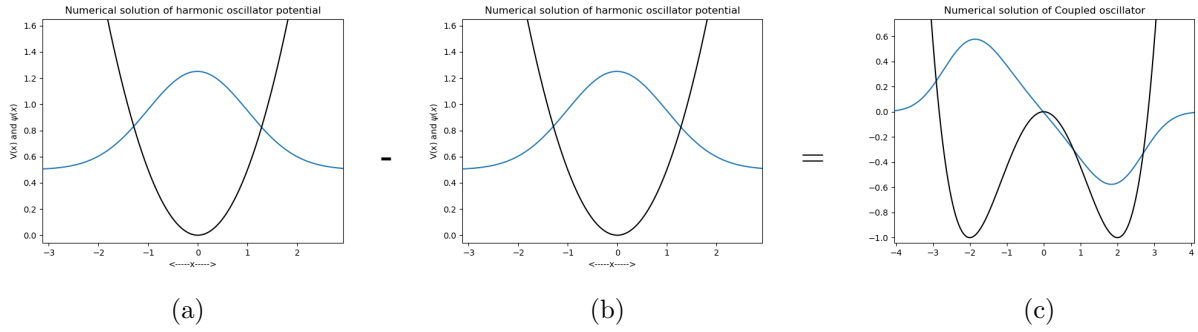


Figure 4: Destructive overlap

The coupled oscillator can be thought of as the perturbation of one harmonic well on another . So initially there should be formation of two degenerate linear combinations [fig-3(c) and fig-4(c)]. But due to perturbation these gets split (from eqn-27) into a higher and a lower level as in fig-2(b). Depending on the level of perturbation the depth and width of the minima in coupled well will vary and extent of splitting of eigenstates will depend on that. Now due to this splitting of degenerate states we are also supposed to deviate from the linear increase of Energy as in harmonic oscillator.

3.3 Energy trends

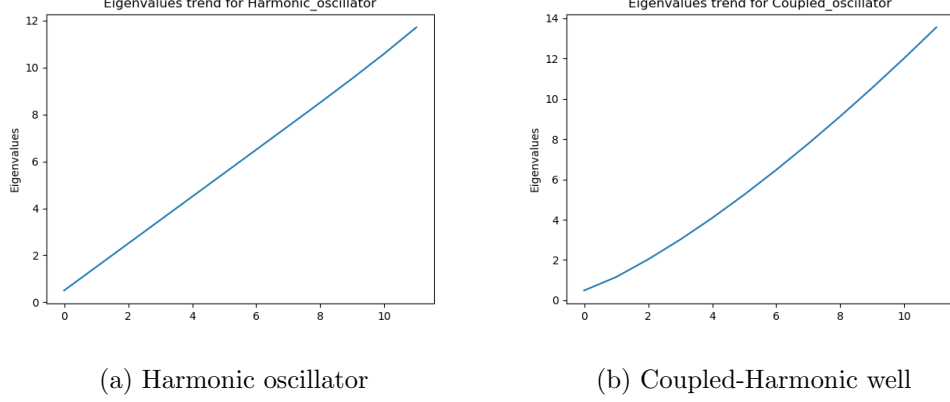


Figure 5: Energy trend of first 10 eigenvalues

As predicted above the Energy levels do not follow a general trend and this happens due to splitting of degenerate energy states by perturbation in coupled oscillator.

3.4 Time-evolution of $\Psi(x, 0)$ in coupled-harmonic well

We start with an initial state which is localised in the left part of the well and let it evolve in time.

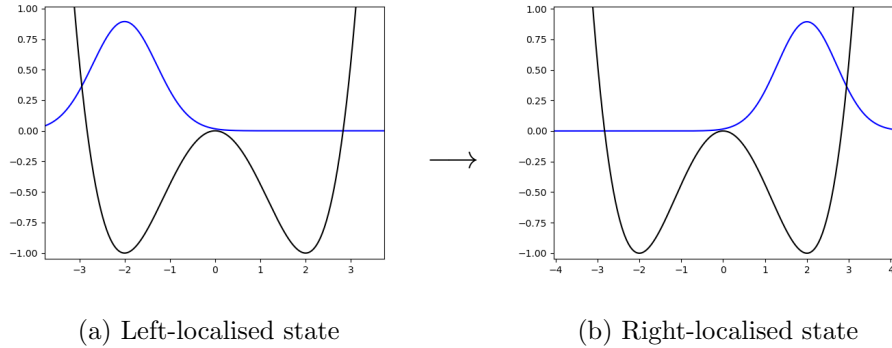


Figure 6: Left localised and right localised states in Coupled-oscillator

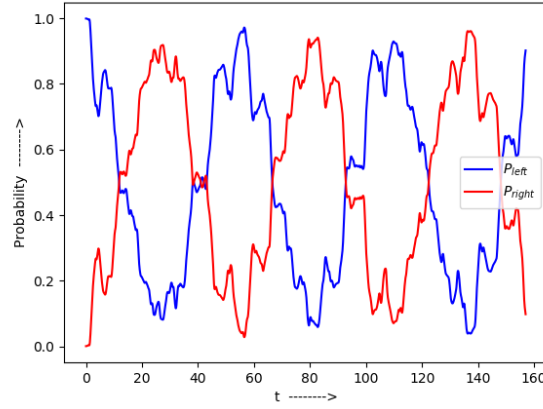


Figure 7: Comparing probability of localising in left and right upon time evolution

As can be seen from fig-7 the particle oscillates between left and right portion of well. This happens as when we try to expand $\Psi(x, 0)$ according to eqn-(15), we will get most contributions from ψ_1 and ψ_2 . This can be seen from fig-1(b) that the initial state resembles most these two states. Now since for both these states there is equal probability of being localised in any of the sides, the initially left localised state oscillates between left and right when evolved through time.

3.5 Asymmetric coupled-harmonic well

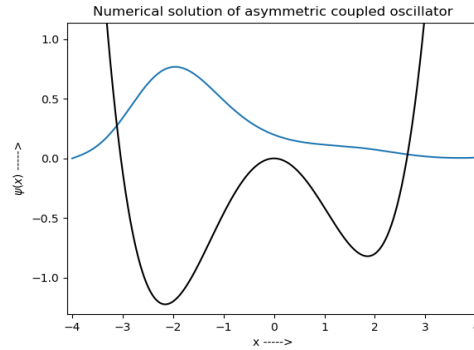


Figure 8: Ground state of asymmetric well with $\gamma = 0.025$

The Asymmetric coupled-harmonic oscillator (given by eqn-14) ground state is localised on the more deeper side as particle feels more attractive force there and thus is tends to get localised there.

3.6 Oscillatory time-dependent perturbation

We now apply an oscillatory time-dependent perturbation of the form $\cos(\omega t)$ on asymmetric-double well. So our new potential looks like

$$V(x, t) = -\frac{2\epsilon}{a^2}x^2 + \frac{\epsilon}{a^4}x^4 + \gamma\cos(\omega t)x^3 \quad (58)$$

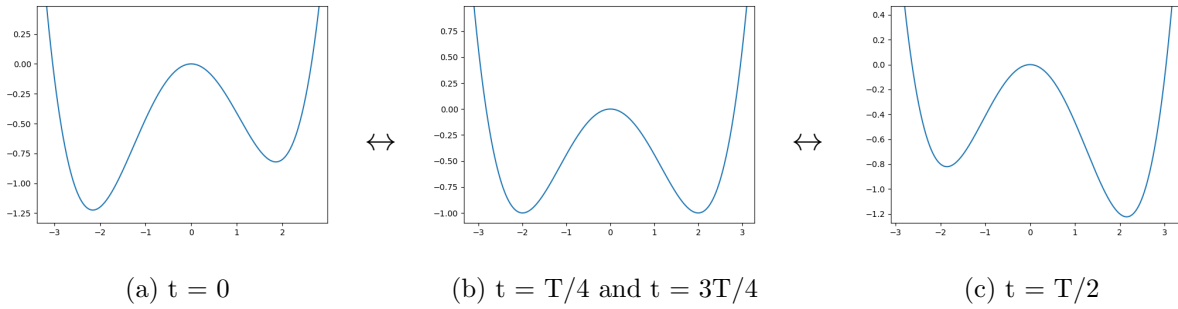


Figure 9: Oscillation of V with time

Depending on the frequency of oscillation ω we can now observe adiabatic and non-adiabatic behaviour of the system. The difference between the first two eigenvalues of system (in eqn-58) with $\epsilon = 1$, $a = 2$ and $\gamma = 0.025$ is calculated to be ≈ 0.1 hartree units. We can thus take this to be near to the natural frequency(ω_0) of the system.

We will now vary ω and try to observe the adiabatic behaviour according to equations (37),(38) and (39). We take the initial state to be the one in fig-8. We then evolve it in time according to eqn(1) by applying the Crank-Nicolson method (section-2.4.2). At each time step we take the projection (c_0 as in eqn-37) of $\psi(x, t)$ on $\psi_{gs}(t_i)$, the instantaneous ground state at $t = t_i$.

3.6.1 When $\omega < \omega_0$

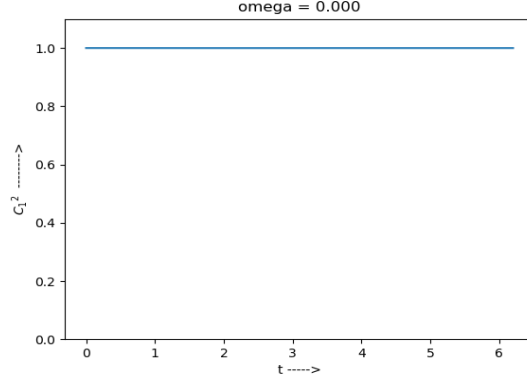


Figure 10: c_1^2 v/s t for $\omega = 0$

This is obvious as $\omega = 0$ implies that there is no time dependent perturbation and the particle remains in its initial state with time.

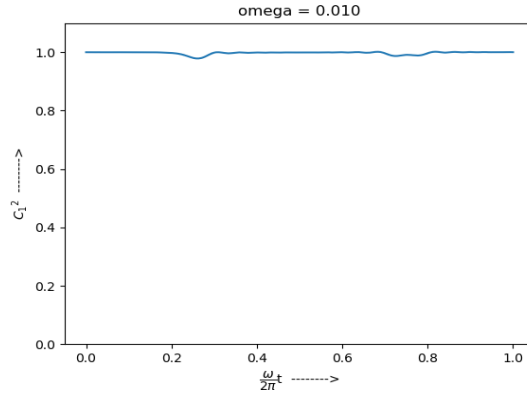
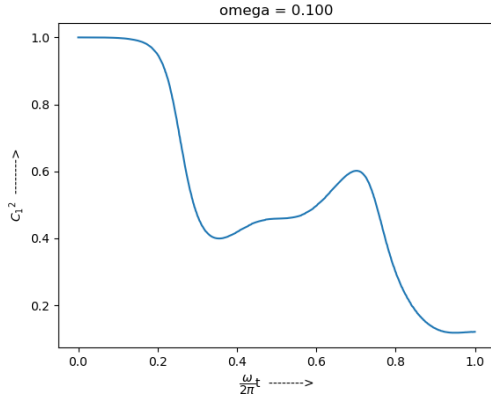


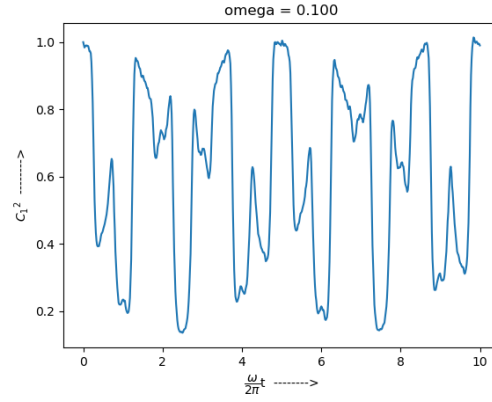
Figure 11: c_1^2 v/s t for $\omega = 0.01$ for 1 time period

We can see clearly at $t = T/4$ and $t = 3T/4$ where the potential goes to fig-9(b), there is a little fluctuation in c_1^2 . But the $c_1^2 \approx 1$ throughout implying that there is little transition to higher state and the process is almost adiabatic.

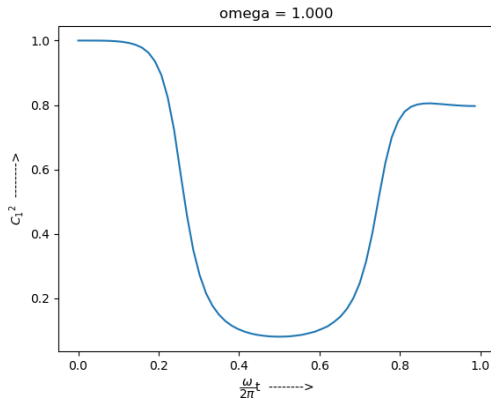
3.6.2 When $\omega \geq \omega_0$



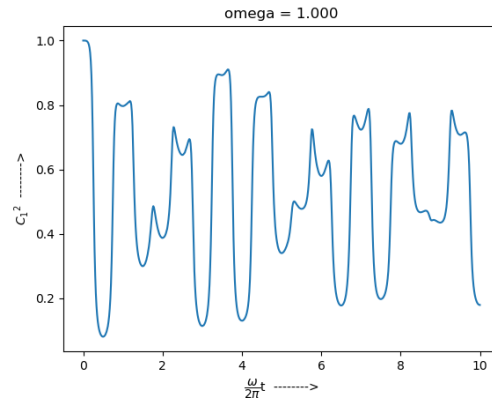
(a) 1 time period



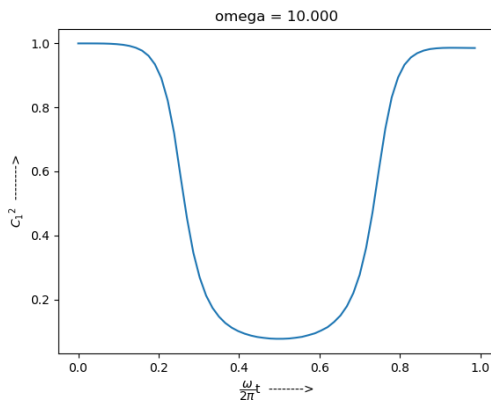
(b) 10 time periods



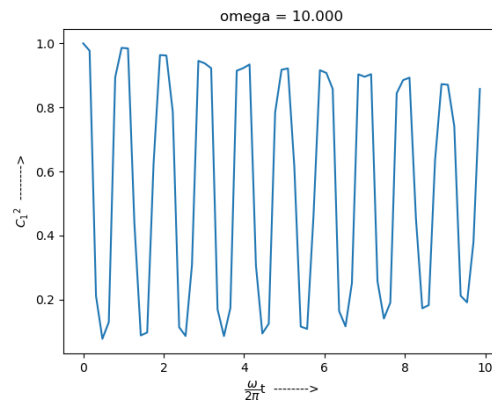
(c) 1 time period



(d) 10 time periods



(e) 1 time period



(f) 10 time periods

Figure 12: c_1^2 v/s t for (a),(b) $\omega = 0.1$;(c),(d) $\omega = 1$;(e),(f) $\omega = 10$

As can be seen as we increase the ω beyond its natural frequency ω_0 then then we see oscillatory changes in c_1^2 which implies that the system makes oscillatory transitions between lower and higher states. This shows the non-adiabatic behaviour as was stated in Adiabatic theorem (section-1.5).

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