One Dimensional Schrödinger Equations

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In the previous chapter, we have developed the wave equation of motion, and we discussed several general properties of the solutions, including normalizability, linearly independent set of possible solutions with discrete energies. Now we will exactly solve for few famous examples in 1D.

(A) Free particle:

Free particle means there is no potential. So, the time-independent Schrödinger equation

$$\hat{H}\psi = \frac{\hat{p}^2}{2m}\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = i\hbar\frac{\partial}{\partial t}\psi(x,t) = E\psi(x,t) \quad -(1)$$

Comparing it with the relativistic wave equation for the electro-magnetic wave (photon), we see that non-relativistic particles have 1st order time-dependence. The general solution remains the same as

$$\psi_k(x,t) = A\,e^{i(kx - \frac{E}{\hbar}t)} + B\,e^{-i(kx - \frac{E}{\hbar}t)} \quad -(2)$$

which consist of two linearly independent solutions in position due to its 2nd order derivative term. The wave vector is easily obtained from eq(1) as

$$E = \frac{\hbar^2 k^2}{2m} \quad --(3)$$

(This is difference from the relativistic wave eq where $E = c\hbar k$).

(One may also write eq (2) instead in terms of $\sin(kx)$ & $\cos(kx)$, but they are the same solutions).

- The energy eigenvalues only depend on k^2, and does not depend on the sign of k, whereas the wavefunctions for $+k$ & $-k$ are linearly independent. This is something new that we have not talked about before. Such solutions are called degenerate solutions.

- A, B are arbitrary constants to be determined. Henceforth, we will only focus on the time independent part where $\Psi(x,t) = \psi(x)\, e^{-iEt/\hbar}$.

- Since E is energy (only kinetic energy), so k is real and the solutions e^{ikx} and e^{-ikx} are always oscillatory in space, i.e., always propagating and never decays even as we go to $x \to \pm\infty$. So, this is going to cause a problem in the normalizibility condition that all wavefunction must follow. Without loosing generality, we only consider one particular solution, say, e^{ikx} and make the k-variable extend to $+k$ to $-k$. Then we have a simpler form to deal with:

$$\psi_k(x) = c\, e^{ikx} \quad \text{---} (4)$$

where c is the constant to be determined. $\pm k$ corresponds to wave travelling right and left directions.

- It is interesting to see that $\psi_k(x)$ is also a simultaneous eigenfunction/ wave function of the momentum operator with momentum eigenvalue $p = \hbar k$ as

$$\hat{p}\psi = -i\hbar \frac{\partial}{\partial x}\psi = p\psi \quad \text{--(5)}_a$$

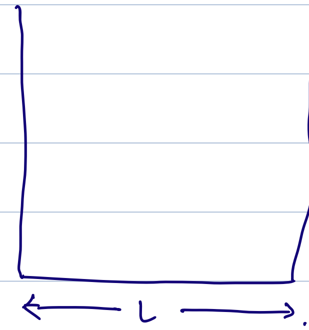
This is obvious also because the Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m}$ commutes with the momentum operator $\hat{p}$. Therefore, in these eigenstates, momentum is fully determined and it has no uncertainty: $\Delta p = 0$. So, position is completely undetermined, $\Delta x \to \infty$, which is expected because the wave is propagating for ever in space and is <u>not</u> <u>normalizable</u>. So, we cannot define its position. Therefore, plane waves are also called momentum eigenstates or simply momentum states.

<u>Normalization</u>: $\int_{-\infty}^{\infty} |\psi|^2 dx = |C|^2 \int_{-\infty}^{\infty} dx \longrightarrow \infty$ --(6).

(Recall that this was the reason we had to invent <u>wave packet</u>, which was to confine the plane waves in a finite size. Practically, this means we have to introduce a confinement at the two boundaries of a length L. This introduces a maximum uncertainty in position to be $\Delta x \to L$ and finite Δp also. The plane waves reflect back at the boundary and create standing waves which are the wave packets.)

- ## Box normalization

For the time being, we will not worry about the confining potential at the boundary of a box, but pretend that the plane wave solutions are only allowed within a length scale of L.



In reality, this should be done by adding a confining potential (called particle in a box) which creates wavepacket, but for the time being we will continue to use plane waves and only restrict the integral from 0 to L. (This is clearly not a physical B.C., but rather a mathematical treatment):

$$\int_0^L |\psi|^2 dx = |C|^2 \int_0^L dx = |C|^2 L. = 1$$

So, $|C| = \frac{1}{\sqrt{L}}$ (we will not worry about the phase part, since any phase in C can be absorbed in ψ due to its constant phase freedom).

So, $$\boxed{\psi(x) = \frac{1}{\sqrt{L}} e^{ikx}} \quad -(7)$$

This is called Box normalization, where $0 \leq x \leq L$. We will see that in the example of particle in a box problem later by setting $V \to \infty$, in which all possible wavefunction $\psi(x)$ have to vanish at the wall which will quantize the possible values of k and energy. (H.W. Estimate k & E for the longest wavelength case using uncertainty principle).

• Periodic Boundary condition :

We imagine there is some periodicity in the system (due to atoms/molecules sitting at lattice sites in solid state systems, etc), so that the wave function must follow the periodic boundary condition :

$$\psi(x+L) = \psi(x) \quad --- \quad (8).$$

$$\Rightarrow \quad c\, e^{ik(L+x)} = c\, e^{ikx}$$

$$\Rightarrow \quad e^{ikL} = 1$$

$$\Rightarrow \quad \boxed{k = \frac{2\pi}{L} n} \quad , \text{ where } n = 0, \pm 1, \pm 2, \cdots .$$

and the normalization condition becomes

$$1 = \int_0^L |\psi|^2 dx = |c|^2 L \quad \Rightarrow \quad c = 1/\sqrt{L}.$$

Now we see that the periodic boundary condition makes k discrete in units of $2\pi/L$ and hence the energy is also discrete

$$E_n = \frac{2\pi^2\hbar^2}{mL^2} n^2 .$$

(• H.W. Is the momentum still conserved or the wavefunction is still a simultaneous wave function of the momentum operator ? Ans: It's conserved modulo $2\pi n/L$).

• Now we see that k or n are the discrete quantum numbers of the wavefunction

$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{i\frac{2\pi n}{L}x} \quad \text{--- (9).}$$

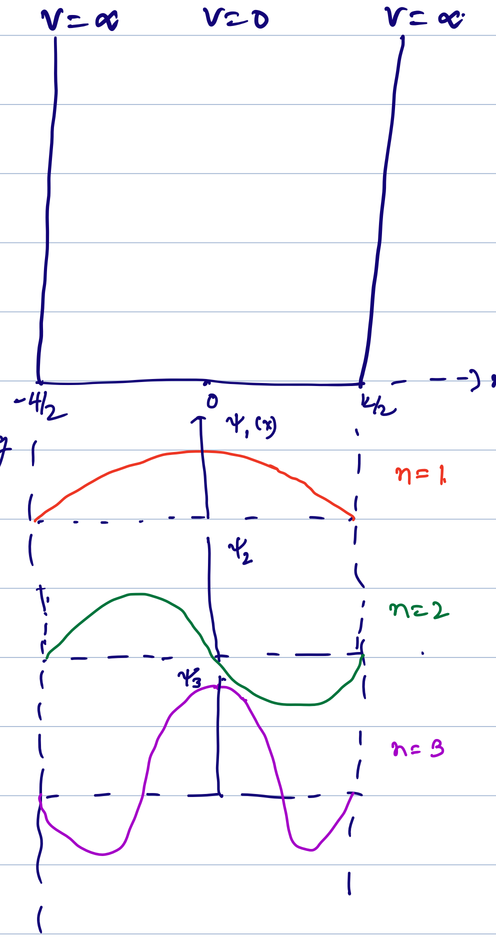
So, different values of k or n corresponding to different, linearly independent eigenfunctions (except $\pm n$ states which are degenerate) and the orthogonal condition becomes.

$$\int_0^L \psi_n^*(x)\, \psi_m(x)\, dx = \frac{1}{L}\int_0^L e^{i\frac{2\pi}{L}x(n-m)}\, dx$$

$$= \delta_{m,n} \quad \text{— (10)}$$

(from the definition of Kronecker delta fn).

(B) Particle in a Box / Infinite Potential Well



Particle in a box is a continuation to the box normalization discussion with completely rigid wall ($V \to \infty$ at $x = \pm L/2$) and $V = 0$ inside $-L/2 < x < L/2$.

Therefore, the probability of finding the particle outside the well is completely zero. Therefore, all possible wavefunctions must vanish at $x = \pm L/2$. Because, the potential inside is zero, so, the solution of the schrödinger equation is still plane waves with the condition that only those plane waves solutions are allowed which have nodes at $x = \pm L/2$. This is to say all the wavelengths (λ) are integer multiple of L as we may have seen in the discussions of wave theory in other courses. Therefore, the condition.

$$\psi_k(\pm L/2) = C\, e^{\pm ikL/2} = 0. \quad -(2)$$

$C = 0$ is a trivial solution. But there are more non-trivial solutions. To find that out we exploit the freedom of choosing the wavefunction (linearly dependent and gauge/phase freedom) to satisfy the boundary condition. In fact, as we will see more and more later, even for a given potential, i.e. the Schrödinger equation of motion, the form of the solution, and hence quantized energy eigenvalues may change if we change the boundary condition. To rewrite the general solution in a form suitable for our boundary conditions, we proceed as

$$\psi(x) = A e^{ikx} + B e^{-ikx}$$
$$= (A+B)\cos kx + i(A-B)\sin kx \quad -(12)$$

Then $\psi(\pm L/2) = 0 \Rightarrow (A+B)\cos\left(\frac{kL}{2}\right) \pm i\,(A-B)\sin\frac{kL}{2} = 0$.

(i) Now we have two choices: $A = -B$, $\sin\left(\frac{kL}{2}\right) = 0$.

$\Rightarrow k = \frac{n\pi}{L}$, $n = 2, 4, 6, \ldots$

(ii) or $A = B$, $\cos\left(\frac{kL}{2}\right) = 0$.

$\Rightarrow k = \frac{n\pi}{L}$, $n = 1, 3, 5, \ldots$

(we do not necessarily have to consider the negative n values since those negative n values are obtained from positive n-values by changing the sign of A, B. So, they are not linearly independent solutions)

Therefore, we have two sets of linearly independent solutions for even & odd integers of n. Therefore, the momenta and hence wavelengths are quantized for a particle in a box and the corresponding quantized energies are

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2} n^2 . \quad --- (18).$$

- Its easy to prove that the eigenstates are orthogonal, and they can be normalized as.

$$\int_{-L/2}^{L/2} dx \; \psi_n^* \psi_m = L .$$

So we divide the eigenstates by $1/\sqrt{L}$ which gives orthonormalized eigenstates.

- **Parity**: We notice that the alternative eigenstates, being $\cos kx$ & $\sin kx$ are even and odd functions of x. This is actually not a coincidence. It actually comes from the symmetry of the Hamiltonian itself. You take all points $x \geq 0$ in the Hamiltonian and invert $x \to -x$, then you see that the potential profile remains unchanged. If the Hamiltonian has a symmetry, then the eigen-states also have the same symmetry. In other words, the eigenstates of the Hamiltonian is also a simultaneous eigenstate of the operator representing that symmetry. This symmetry is called parity. Lets say P is the symmetry operator whose job is to invert the position variable x to $-x$ in the eigenstate.

So, P is defined as $P\psi_n(x) = \psi_n(-x)$. ---- (14).
(Don't look for any mathematical form of the P operator. Its an abstract operator whose job is to invert all x to −x.) Then apply P again on Eq (14) to obtain

$$P^2\psi_n(x) = P\psi_n(-x) = \psi_n(x).$$

So, $\psi_n(x)$ is an eigenstate of P^2 with eigenvalue 1. Since P is an Hermitian operator whose eigenvalues are real, so, the eigenvalues of P can be ±1. So, we get

$$P\psi_n(x) = \psi_n(-x) = \pm\psi_n(x).$$

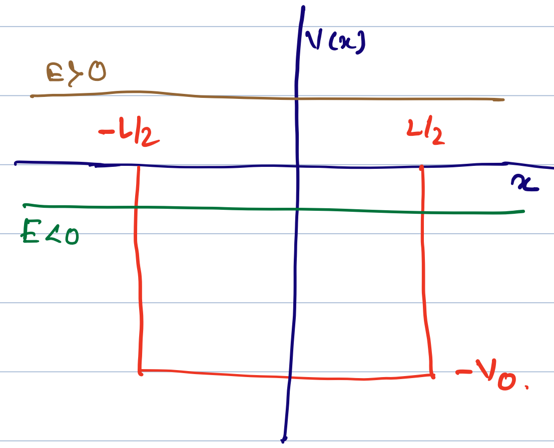
where +1 & −1 eigenvalues correspond to the even & odd values of n. Therefore, owing to the parity symmetry of the Hamiltonian, the eigenfunctions are also eigenfunctions of the parity operator and hence each eigenstate have well defined parity (either even or odd in spatial inversion). If a Hamiltonian does not have the parity, i.e. spatial inversion symmetry then the eigenfunctions also don't have this symmetry, as the eigenstates are not purely odd or even in spatial inversion, but a linear combination of them.

H.W. 1. Assume the potential is now shifted to $V=\infty$ at $x=0$ & L and $V(x)=0$ for $0<x<L$. Does this system have parity?

2. Estimate the ground state energy of the Hamiltonian, ie, $E_1 = \frac{\hbar^2 \pi^2}{2m L^2}$ from the uncertainty principle.

3. Extend the calculation to 3D. Find the degeneracy in each energy levels.

(c) Finite Potential well

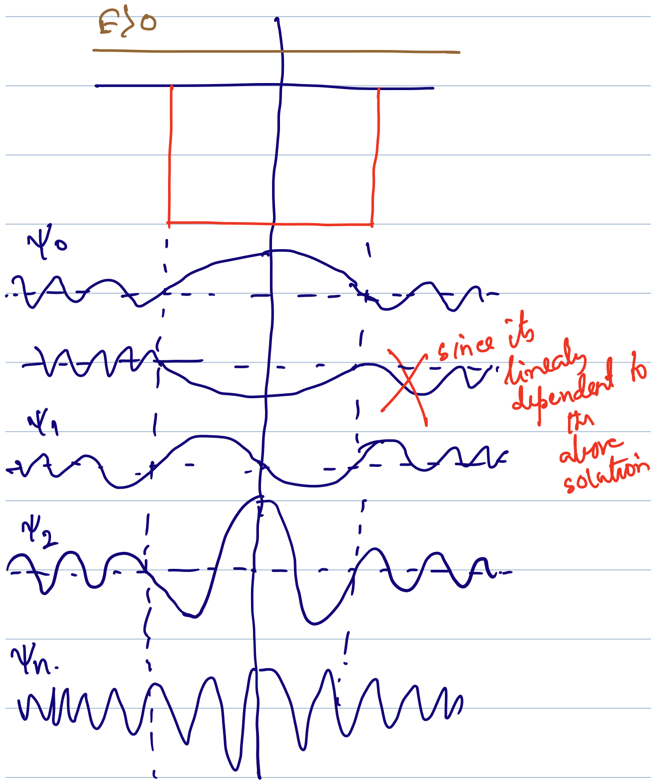


Next we will consider a finite potential well (means negative potential). Although this is more of an idealized potential profile, but the conclusions drawn here are qualitatively similar to the Yukawa potential profile (attractive potential). We are interested in two energy solutions $E > 0$ and $-V_0 \leq E < 0$. The solution of the first case is easy to guess that because of the positive kinetic energy, the solutions will be plane wave like with slight modification due to the potential. Such solutions are called scattering solution, because as if a free particle is being scattered by the potential well (although, one might say here that the particle is being attracted towards the potential well). Then the question would be can the particle avoid the attractive potential and jump to the other side or become trapped at the well? Clearly it depends on the potential height $-V_0$, and width L.

The $E < 0$ situation is interesting. Outside the well, we have negative K.E., and inside the well, positive K.E. So, the solutions will be decaying outside the well (classically forbidden region) and oscillatory inside the well. Each oscillation with different wavelength which corresponds to linearly independent solutions will have different quanta of energy which are the energy eigenvalues.

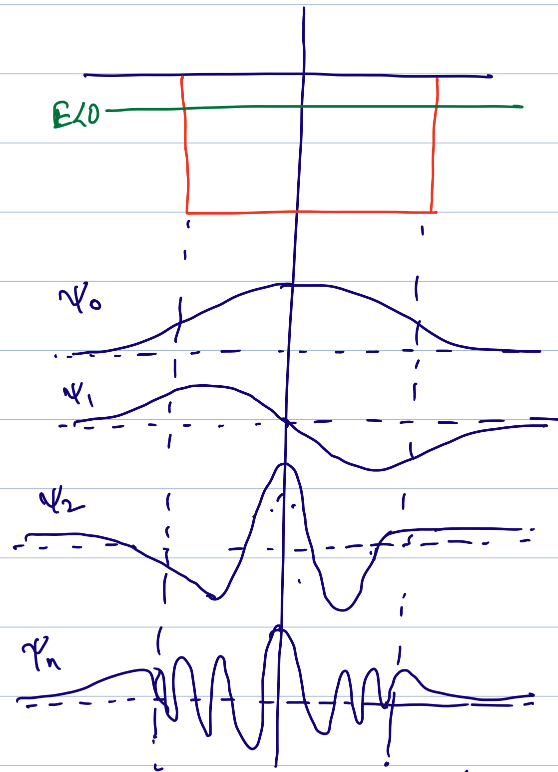
So larger wavelength (or spread of the wave packet) correspond to lower energy or the other way? Its mostly the wave packet with larger spread / uncertainty in position and hence less spread in momenta correspond to the lower energy states. The ground state often reaches the optimum uncertainty $\Delta p \Delta x \sim \hbar$. (One should not take this condition blindly in the future courses since for complicated potential profile, and also when potential depends on momentum, like a charge particle in a magnetic field, things can start looking differently, although ground state having optimum uncertainty $\Delta p \Delta x \sim \hbar$ is very much the case in most cases).

- Because the potential, and hence the Hamiltonian has inversion ($x \to -x$) symmetry, so all eigenstates will have definite parity. The ground state wave function will have one maximum at $x=0$ (where the probability density should be maximum. So, we can sketch the wave functions in both cases as follows:



Inside wave packet, outside plane wave like.

Can we do the same here?



Inside wave packet, outside decaying solution.

We can use the uncertainty principle to estimate the ground state energy.

C1 $-V_0 \leq E \leq 0$.

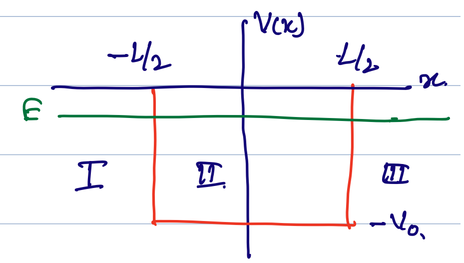
Now we return back to solving the Schrödinger equation exactly. We first consider the $-V_0 \leq E \leq 0$ case.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\,\psi(x) = E\,\psi(x).$$

$$\Rightarrow \quad \frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}\left(V_0 + E\right)\psi(x). \quad \text{--(1)}$$

Lets put $V_0 > 0$ & $E = -|E|$

We have three regions I, II, III where the potential profiles are well defined and we have exact solutions. At the boundaries the potential rises sharply. So, instead of solving at the boundary, we will use the boundary condition of continuity of wave function and its first derivative to obtain its value at the boundary.



Region I, $x < -L/2$ }
Region III, $x > L/2$ } $V(x) = 0$, $E = -|E|$.

$$\frac{d^2\psi}{dx^2} = -\frac{2m|E|}{\hbar^2}\psi(x)$$

$$= -\kappa^2\,\psi(x). \quad \text{- (2).}$$

where $\kappa = \sqrt{\dfrac{2m|E|}{\hbar^2}}$ --(3)

(κ has the dimension of inverse length, so its associated with decaying length scale of the wave packet and uncertainty).

So, the general solutions are :

$$\psi_I(x) = A e^{-Kx} + B e^{Kx}$$
$$\psi_{III}(x) = C e^{-Kx} + D e^{Kx}$$

[No 'i' in exponent].

As $x \to -\infty$ in region I, e^{-Kx} blows up. So, to have normalization condition satisfied, $A = 0$. Similarly $D = 0$. So, we have.

$$\psi_I(x) = B e^{Kx} \quad \text{--- (4a)}$$
$$\psi_{III}(x) = C e^{-Kx} \quad \text{--- (4b)}$$

Because of parity ie, $\psi_I(x) = \psi_{III}(-x)$. This says $\boxed{B = C}$.

Region II :
$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(|V_0| - |E|)\,\psi(x) \quad \geq 0.$$
$$= k^2\,\psi(x) \quad \text{where } k = \sqrt{\frac{2m(|V_0|-|E|)}{\hbar^2}}.$$

General solution is

$$\psi_{II}(x) = E' e^{ikx} + F' e^{-ikx}$$

This solution does not have a well defined parity. Since the potential profile is symmetric under inversion, so we anticipate that all solutions will be either even or odd under parity (in fact alternative solutions will be even & odd). So its convenient to write in the $\sin(kx)$ & $\cos(kx)$ form.

$$\psi_{II}(x) = E\cos kx + F\sin kx. \quad \text{--(4c)}$$

For alternating eigenstates, E & F are expected to be zero.

- We will evaluate the coefficients B, C, E, F by the boundary conditions.

(i) $$\psi_I(-L/2) = \psi_{II}(-L/2)$$

$$\Rightarrow \quad B\, e^{-\kappa L/2} = E \cos\left(\frac{kL}{2}\right) - F \sin\left(\frac{kL}{2}\right). \qquad \text{--- (5a)}$$

(ii) $$\psi_{II}(L/2) = \psi_{III}(L/2)$$

$$\Rightarrow \quad E \cos\left(\frac{kL}{2}\right) + F \sin\left(\frac{kL}{2}\right) = B\, e^{-\kappa L/2} \qquad \text{--- (5b)}$$

(iii) $$\left.\frac{d\psi_I}{dx}\right|_{x=-L/2} = \left.\frac{d\psi_{II}}{dx}\right|_{x=-L/2}$$

$$\Rightarrow \quad \kappa B\, e^{-\kappa L/2} = E \sin\left(\frac{kL}{2}\right) + F \cos\left(\frac{kL}{2}\right) \qquad \text{--- (5c)}$$

(iv) $$\left.\frac{d\psi_{II}}{dx}\right|_{x=L/2} = \left.\frac{d\psi_{III}}{dx}\right|_{x=L/2}$$

$$\Rightarrow \quad -E \sin\left(\frac{kL}{2}\right) + F \cos\left(\frac{kL}{2}\right) = -\kappa B\, e^{-\kappa L/2} \qquad \text{--- (5d).}$$

- For even eigenstate: $F=0 \Rightarrow$ $\boxed{\kappa = k \tan\left(\frac{kL}{2}\right)}$ --- (6a)
- For odd eigenstate: $E=0 \Rightarrow$ $\boxed{\kappa = -k \cot\left(\frac{kL}{2}\right)}$ --- (6b).

- Eqs. (6a) & (6b) put constraints on the allowed values of the plane wave solutions, i.e, on the values of k separately for the even and odd state. Typically a plane wave solution has continuous values of k and hence, continuous energy. But as a boundary condition is imposed, only certain set of discrete k-values become allowed which for wavepacket with uncertainty in position which is of the order of the width of the potential well L. In fact the spread of the wave packet is encoded in the parameter κ. Notice that κ has the dimension of length inverse. It roughly gives us a length scale where the wave packet vanishes outside the well. Therefore, the $\hbar/\Delta x = \hbar\kappa$ then gives us the spread of momentum across its mean wavevector. We can see that easily for the ground state.

The ground state corresponds to large wavelength, i.e., small wavevector k. For $k \to 0$, $\tan(kL/2) \sim kL/2$. Hence from eq (6a) we get $\kappa \approx k^2 L/2$. Now, the K.E. of the particle is $\frac{\langle p^2\rangle}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \kappa}{mL}$. Now, the average momentum of the particle in the ground state is zero. So, the uncertainty in momentum $\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\langle p^2\rangle} \sim \hbar\sqrt{\frac{2\kappa}{L}}$. Therefore, the uncertainty in position is $\Delta x \sim \pi\sqrt{\frac{L}{2\kappa}}$. Since the maximum uncertainty in the ground state is of the order of L, hence $\kappa \sim \frac{\pi^2}{2L}$.

From here we can also estimate the ground state energy as follows. We know that

$$V_0 - |E| = \frac{\langle p^2\rangle}{2m} = \frac{(\Delta p)^2}{2m} \sim \frac{\hbar^2 \kappa}{mL} = \frac{\pi^2\hbar^2}{2mL^2}$$

$$\frac{h}{2\Delta x} = \frac{h}{2\pi}\cdot\sqrt{\frac{2\kappa}{L}}, \quad \Delta x = \pi$$

Therefore

$$\boxed{|E| - V_0 = -\frac{\pi^2\hbar^2}{2mL^2}} \quad \text{---} (7)$$

We will see below that this ground state energy matches with the exact calculation.

(*) **Energy eigenstates:** Our next step is to solve eqs (6a) and (6b) and find out the values of k and hence the energy eigenvalues which are the allowed solutions. It's not possible to solve eqs (6a), (6b) analytically. The idea is at what values of energy E, the R.H.S. & L.H.S match. For that we can plot $k\tan(kL/2)$ vs E and κ vs E and their intersection points give the even eigenvalues. Similarly for the odd solutions.

From eq (6a),

$$\tan\left(\frac{kL}{2}\right) = \frac{\kappa}{k} = \frac{1}{k}\sqrt{\frac{2m}{\hbar^2}V_0 - \frac{2m}{\hbar^2}|E|}$$

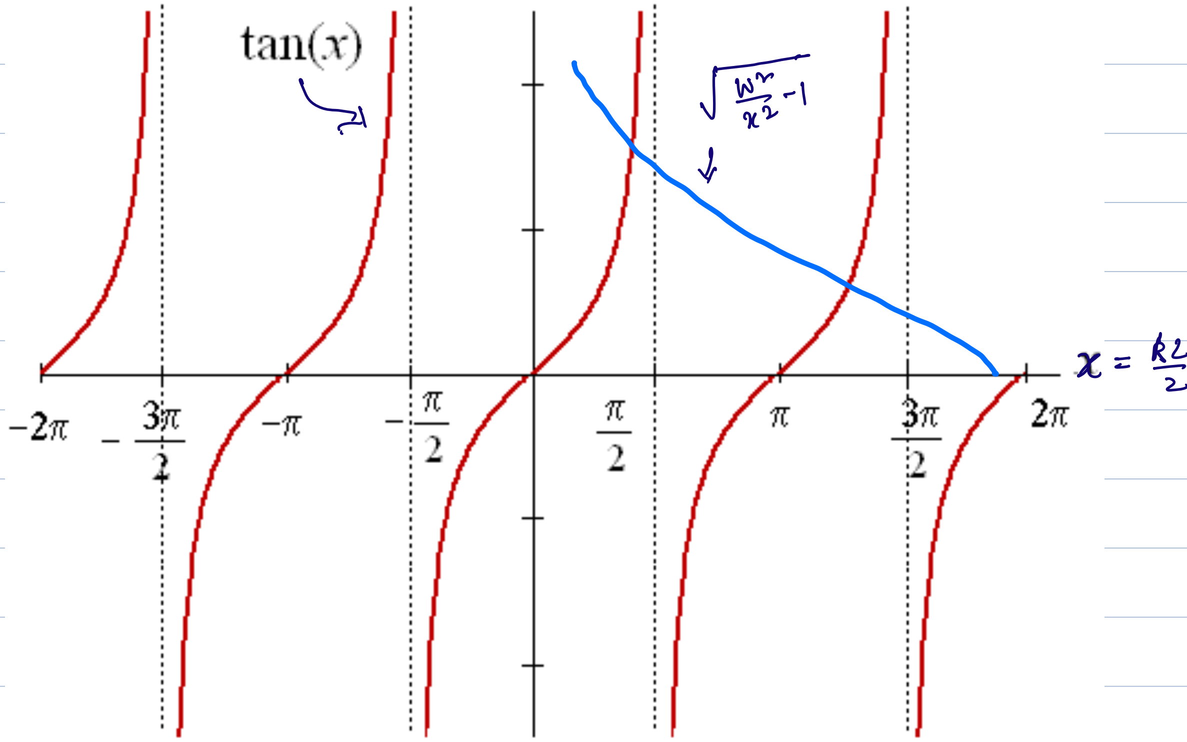
$$= \frac{1}{k}\sqrt{\frac{2mV_0}{\hbar^2} - k^2}$$

$$= \sqrt{\frac{2mV_0}{\hbar^2 k^2} - 1}$$

$$= \sqrt{W^2\left(\frac{2}{kL}\right)^2 - 1} \quad \text{---} (8)$$

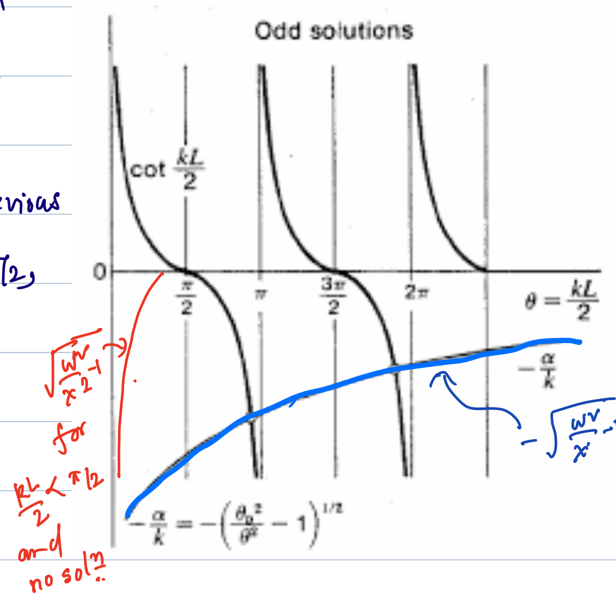
where $W = \sqrt{\frac{mV_0L^2}{2\hbar^2}}$ is a dimensionless parameter depends on system (V_0L^2) and particle mass.

We know that $\tan x$ is a trancendental function defined between $\frac{n\pi}{2} < \tan x \leq \frac{(n+1)\pi}{2}$, for n = integer, and $x = kL/2$. A plot of R.H.S $= \sqrt{\frac{W^2}{x^2} - 1}$ is shown by blue line. Therefore, depending on the values of W, the R.H.S. function crosses only certain positive integer number of $\tan x$ which gives the finite number of quantized energy. We notice that R.H.S vanishes at $x = \frac{kL}{2} = W \Rightarrow k = \sqrt{\frac{2mV_0}{\hbar}}$ which puts the



upper limit on the wave vector k. We notice that as $x \to 0$, $\tan x \to x$ and $\sqrt{\frac{W^2}{x^2}-1} = \tan x \approx x$. So we have $W^2 = x^2(1+x^2)$, both sides have the same sign, therefore, there will always be at least one solution no matter how small k. This means, there will always one bound state solution in a potential well, such that the particle will be confined inside the well and the wavefunction will die off fast. We will see that by going to the narrow potential well limit below. But even for a bound state, the wave function spreads outside the potential well and the probability of finding the particle outside the well is finite (which will not be the case for a classical particle).

- For odd parity solutions, we have the similar result. We see that it is defined between $n\pi$ to $(n+1)\pi$ and hence it takes the odd integer if we rewrite in the previous form. If we make $kL/2 < \pi/2$, the R.H.S misses to cross the $\cot(kL/2)$ line and hence no energy solution. This is the reason the odd parity solution does not give a ground state solution, but it gives the first excited state and all odd parity excited states.



(*) Summery : For $E<0$, we have two regions. Inside the pot. well, K.E. is positive and we have scattering / oscillatory wave with wavevector k. Outside the well, we have −ve K.E and hence decaying wave with decay length κ^{-1}. Continuity of w.f. and and derivative gives a relation between k & κ, saying not all wavevectors are possible and that restriction quantizes energy. Small k, i.e., larger wavelength always correspond to lower energy. Ground state has highest wavelength and 1st excited state has smaller wavelength and so on. In all cases, the w.f spread out of the well, implying that the particle has finite probability of simultaneously being outside the well.

(*) We can take two limits here. (Ref: Marzbecker ch 6)

I. Wide & Deep Well: We first consider $V_0 \to \infty$ limit with L remaining finite. This makes $W \to \infty$. In this case the R.H.S. $\sqrt{W^2/x^2 - 1} \to \infty$. On the L.H.S, we have $\tan x \to \infty$ as $x \to (n+1)\pi/2$. This quantizes k as $\frac{k_n L}{2} = (n+1)\pi/2$.

Therefore, we get:

$$V_0 - |E_n| = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2m} \cdot \frac{(n+1)^2 \pi^2}{L^2}$$

$$\text{or} \quad \boxed{|E_n| - V_0 = -(n+1)^2 \frac{\hbar^2 \pi^2}{2mL^2}} \quad \cdots (9)$$

$n = 0, 2, 4, \cdots$

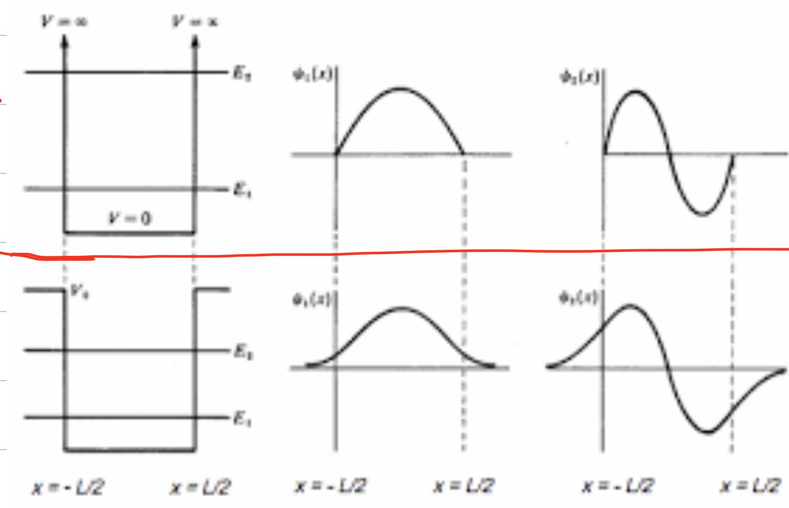
(Books write it as $E + V_0 = n^2 \frac{\hbar^2 \pi^2}{2mL^2}$, where E is assumed to be −ve. I have just substituted $E = -|E|$ and n runs from $1, 3 \cdots$)

- Remarkably, $n=0$, the ground state solution matches well with the result obtained in eq (7) using the uncertainty principle.

Wave functions.:

Infinite pot. well

Finite pot. well



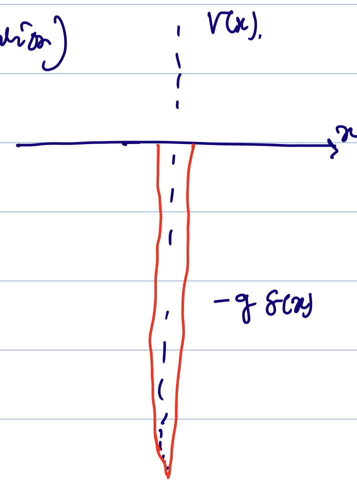
We see that as we increase V_0, the decay length κ^{-1} decreases, this means the spread of the wavefunction keeps on decreasing and the wave function becomes confined inside the potential well and hence we reproduce the results from our previous example.

II. Delta function potential:

Another interesting limit is to take $V_0 \to \infty$ while at the same time $L \to 0$ such a way that the area under the potential curve, i.e, $\boxed{V_0 L = g}$ remains finite. This actually takes us to the delta function potential limit as

$$V(x) = - \lim_{\substack{V_0 \to \infty \\ L \to 0}} \left(V_0 L \right) = - g\, \delta(x). \qquad \text{--} (10)$$

(watch out the problem with dimension)



- In this limit $kL/2 \to 0$.

So, in the $\tan\left(\frac{kL}{2}\right) \sim \frac{kL}{2}$, the R.H.S still crosses the first $\tan\left(\frac{kL}{2}\right)$ line, and we have <u>one bound state</u>, but no excited states because $\cot(kL/2)$ line is not crossed by the $-\sqrt{\frac{w^2}{x^2} - 1}$ line. The bound (ground) state energy can still be estimated from the same uncertainty principle. In the $k \to 0$ limit, from eq(6a): $K \approx k \tan\left(\frac{kL}{2}\right) \to k^2 L/2$.

Now, $w^2 = \frac{m V_0 L^2}{2\hbar^2} = \frac{k^2 L^2}{4} \Rightarrow \frac{k^2 L}{2} = \frac{m V_0 L}{\hbar^2} = \frac{mg}{\hbar^2}$.

So, $K = mg/\hbar^2$. This gives:

$$E = -\frac{\hbar^2 K^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{mg}{\hbar^2}\right)^2 = -\frac{m g^2}{2\hbar^2} \qquad \text{--} (11)$$

Thus the attractive 1D delta function supports only one bound state which is the ground state energy.

- We can also obtain this result from full calculations. The Schrödinger equation is

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}\left(E + g\delta(x)\right)\psi(x) \quad \text{---(12)}$$

We continue to call region I $(x<0)$ & region III $(x>0)$ whereas where region II is now a line.

In both regions I & III, we have $V(x)=0$ & $E=-|E|$,

so,
$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}|E|\,\psi = -k^2\psi \quad \text{---(13)}$$

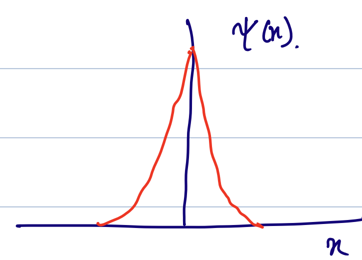
where $k = \sqrt{\frac{2m|E|}{\hbar^2}}$, corresponding to the inverse decay length.

Solutions in two regions are

$$\psi_I(x) = A e^{-kx} + B e^{kx}, \text{ for } x<0, \quad \text{---(14a)}$$
$$\psi_{III}(x) = C e^{-kx} + D e^{kx}, \text{ for } x>0. \quad \text{---(14b)}$$

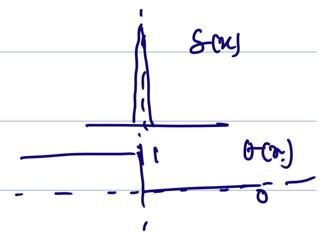
- clearly $Ae^{-kx} \to \infty$ as $x \to -\infty$ and $De^{kx} \to \infty$ as $x \to \infty$. So, for the wavefunctions to be normalizable, A & D have to vanish.
- $\psi(x)$ is continuous at $x=0$. This gives $B=C$.

So, we get $\psi_{I,III}(x) = B\, e^{\pm kx}$ --(15)



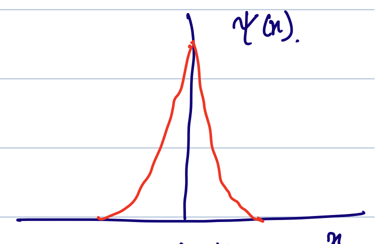
- But here the difference is that the first derivative of the wave function is discontinuous (a step function). Because its 2nd derivative, following the Schrödinger equation has a singularity (divergence) at $x=0$. Since we know that a delta function can also be denoted by the derivative of a step function, so, we can anticipate that as we remove a derivative term from the Schrödinger equation, we will get the step function. So we can write

$$V(x) = -g\,\delta(x) = -g\,\frac{d\theta}{dx},$$



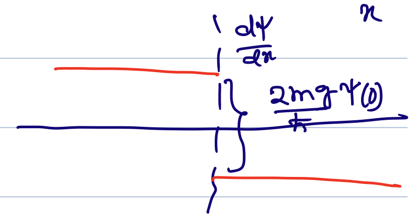
Then we integrate both sides of the Schrödinger equation from $-\infty$ to $-\varepsilon$ & $+\varepsilon$ to $+\infty$, where ε is an infinitesimal number. This gives

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}\left(E + g\,\delta(x)\right)\psi.$$



$$\boxed{\lim_{\varepsilon\to 0} \left.\frac{d\psi}{dx}\right|_{-\varepsilon}^{\varepsilon} = \frac{2mg}{\hbar^2}\,\psi(0)} \quad \text{--- (16)}$$

From eq (15), we get



$$\left.\frac{d\psi}{dx}\right|_{x=0} = 2BK\, e^{+Kx}\Big|_{x=0}$$

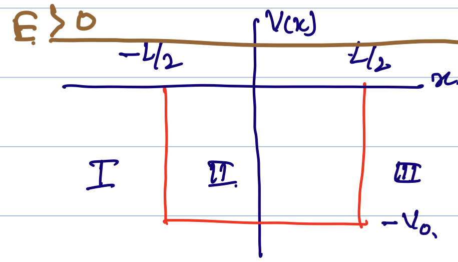
$$= 2K\,\psi(0) \quad \text{--- (17)}$$

Therefore, from eq (16) & (17) we get $\boxed{K = \frac{mg}{\hbar^2}}$

Then the ground state energy is

$$\boxed{E = -\frac{\hbar^2 K^2}{2m} = -\frac{m g^2}{2\hbar^2}} \quad \text{-(18)}$$, which is same as Eq (1).

C2 For $E > 0$.



In this case, the kinetic energy of the particle is always positive, with an increase in kinetic energy in region II. Therefore, the problem can be thought of as a scattering problem (particle-like behavior of a plane wave) in which the potential well serves as a scatterer which gives/removes energy of the particle.

In region I & III, we have free particles whose solutions are

$$\psi_I(x) = A e^{ikx} + B e^{-ikx} \quad --(1)$$

$$\psi_{III}(x) = C e^{ikx} + D e^{-ikx} \quad --(2)$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$

In region II, we have

$$\frac{d^2}{dx^2}\psi_{II}(x) = \frac{2m}{\hbar^2}(-V_0 - E)\psi_{II}(x)$$

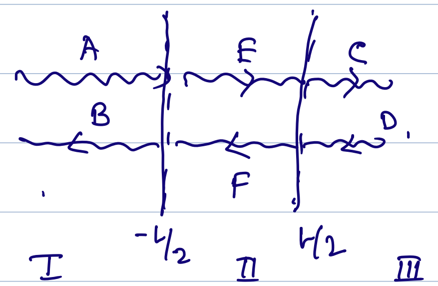
$$= -k'^2 \psi_{II}(x)$$

$$\Rightarrow \psi_{II}(x) = E e^{ik'x} + F e^{-ik'x} \quad ----(3)$$

where $k'^2 = \sqrt{\frac{2m(E+|V_0|)}{\hbar^2}}$

So, all three solutions are oscillatory.

The interpretations of the coefficients A, B, C, D, E F are as follows. A is the amplitude of an incoming wave, and B is the amplitude of the reflected wave from the potential well. E, F, C & D follow similarly.



We will not be interested in the eigenvalue problem here. Rather the present interest is a scattering problem. We start with an incoming wave with amplitude A, and C is the outgoing or <u>transmitted</u> wave from the scattering potential, while B is the amplitude of the reflected wave. For such an initial condition, D = 0, and the relation between C and A, B will be bridged by E & F and the wavevectors k', k.

To figure out the relations, we employ the boundary condition, i.e., the continuity of the wave function and its derivative at the two walls.

- At $x = -L/2$:
  - $\psi_{I}(-L/2) = \psi_{II}(-L/2)$

$$\Rightarrow A e^{-ikL/2} + B e^{ikL/2} = E e^{-ik'L/2} + F e^{ik'L/2}. \quad \text{--- (4a)}$$

  - $\left.\dfrac{d\psi_{I}}{dx}\right|_{x=-L/2} = \left.\dfrac{d\psi_{II}}{dx}\right|_{x=-L/2}$

$$\Rightarrow A e^{-ikL/2} - B e^{ikL/2} = \frac{k'}{k}\left(E e^{-ik'L/2} - F e^{ik'L/2}\right) \quad \text{--- (4b)}$$

Define $k_{\pm} = \frac{1}{2}(k \pm k')$, $\theta_{\pm} = k_{\pm} L$

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{k} \begin{pmatrix} k_+ e^{i\theta_-} & k_+ e^{i\theta_+} \\ k_- e^{-i\theta_+} & k_+ e^{-i\theta_-} \end{pmatrix} \begin{pmatrix} E \\ F \end{pmatrix} \quad \text{---} (5).$$

(H·W)

- At $x = L/2$:
  - $\psi_{II}(L/2) = \psi_{III}(L/2)$

$$\Rightarrow E\, e^{ik'L/2} + F\, e^{-ik'L/2} = C\, e^{ikL/2} + D\, e^{-ikL/2} \quad \text{--} (6a)$$

  - $\left.\dfrac{d\psi_{II}}{dx}\right|_{x=L/2} = \left.\dfrac{d\psi_{III}}{dx}\right|_{x=L/2}$

$$\Rightarrow E\, e^{ik'L/2} - F\, e^{-ik'L/2} = \frac{k}{k'}\left(C e^{ikL/2} - D e^{-ikL/2}\right) \quad \text{---} (6b).$$

$$\Rightarrow \begin{pmatrix} E \\ F \end{pmatrix} = \frac{1}{k'} \begin{pmatrix} k_+ e^{i\theta_-} & k_- e^{-i\theta_+} \\ -k_- e^{i\theta_+} & k_+ e^{-i\theta_-} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \quad \text{--} (7).$$

Combining eqs (5) and (7), we get

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \quad \text{--} (8)$$

where

$$M_{11} = M_{22}^* = \left(\cos k'L - \frac{i\varepsilon}{2}\sin k'L\right) e^{ikL} \quad \text{---} (9a)$$

$$M_{12} = M_{21}^* = \frac{i\eta}{2}\sin k'L. \quad \text{---} (9b).$$

where $\varepsilon = \dfrac{k'}{k} + \dfrac{k}{k'}$, $\eta = \dfrac{k'}{k} - \dfrac{k}{k'}$.

- As we mentioned, we assume the case where a wave is incident from the left and there is no wave incident from right. So, $D=0$.

Then we get

$$\frac{C}{A} = \frac{1}{M_{11}} = \frac{e^{-ikL}}{\cos k'L - \frac{i\varepsilon}{2}\sin k'L} \quad \text{--- (10a)}$$

$$\frac{B}{A} = \frac{M_{21}}{M_{11}} = \frac{i\eta}{2} \frac{\sin k'L \, e^{-ikL}}{\cos k'L - \frac{i\varepsilon}{2}\sin k'L} \quad \text{--- (10b)}$$

Now recall our definition that A is the incident wave amplitude, while C & B are the transmitted and reflected waves. Therefore, the transmission & reflection coefficients are defined as

$$T = \frac{|C|^2}{|A|^2} \; ; \quad R = \frac{|B|^2}{|A|^2} \quad \text{--- (11)}.$$

[H.W. show that $|T| + |R| = A^2$.].

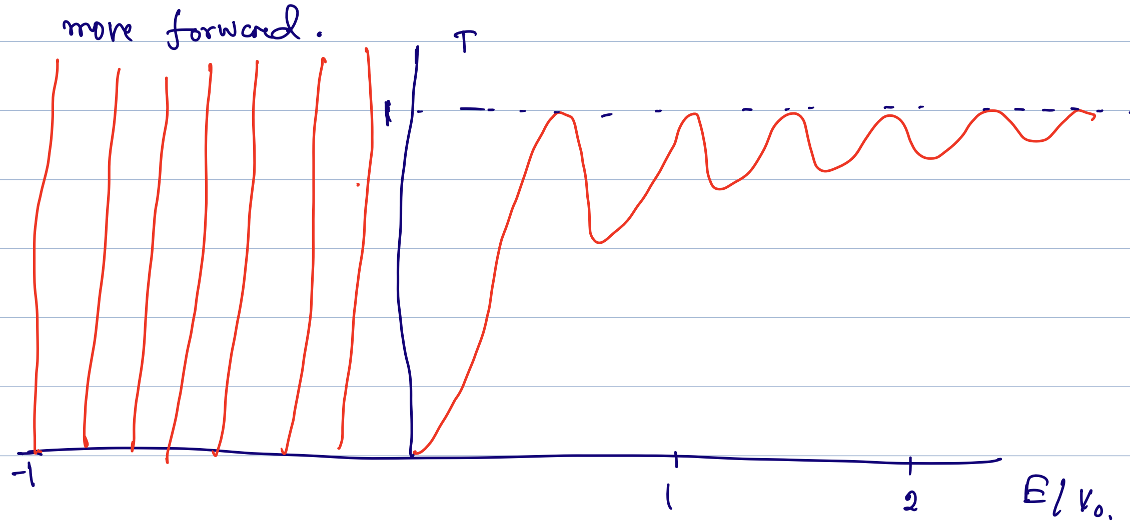
- $$T = \frac{1}{\cos^2 k'L + \frac{\varepsilon^2}{4}\sin^2 k'L}$$

$$= \left[1 + \frac{V_0^2 \sin^2 k'L}{4E(E+V_0)}\right]^{-1} \quad \text{--- (12a)}$$

$$R = \frac{\eta^2}{4} \frac{\sin^2 k'L}{\cos^2 k'L + \frac{\varepsilon^2}{4}\sin^2 k'L}$$

$$= \left[1 + \frac{4E(E+V_0)}{V_0^2 \sin^2(k'L)}\right]^{-1} \quad \text{--- (12b)}$$

• We notice that $T < 1$, which is in contradiction to the expected classical result in which the particle should fully move forward.



• Clearly, transmission starts as $E > 0$. With increasing energy, the transmission probability oscillates sharply at the begining with the maximum value reaching at $T = 1$. From eq(12a), we see that maximum transmission occurs when $\sin k'L = 0$, i.e.

$$k'L = n\pi, \qquad n = 1, 2, 3, \ldots$$

This condition is satisfied when the wave 'E' and the reflected wave 'F' are completely out of phase (differ by $n\pi$ phase), they have an descructive interference. Therefore, the wave can not reflect from the wall at $x = L/2$, and the wave pass through the well. This is some times called <u>anti-localization</u>, in the sense that when a particle looses its momentum via scattering, it is said to be localized. But here .

due to destructive interference, no scattering or localization occurs. We can find out the energy levels of the well as

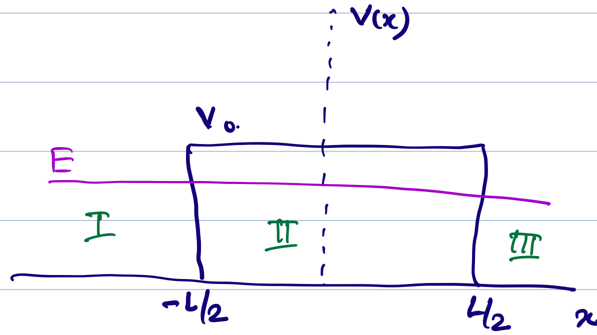
$$E + V_0 = \frac{\hbar^2 k'^2}{2m} = \frac{\hbar^2 \pi^2}{2m L^2} n^2 .$$

- The minimum transmission occurs when $k'L = n\pi/2$.

- As $E \to \infty$, we reach the classical limit where $T \to 1$.

- As $V_0 \to \infty$, the transimission coefficient $T \to 0$ as we can infer from eq 12(a). However, as the resonance condition $k'L = n\pi$ is reached, the potential term exactly vanishes and we have a complete reflection.

(D) Potential Barrier & Quantum Tunneling



Next we consider a finite potential barrier as defined by $V(x) = V_0 > 0$ for $-L/2 < x < L/2$

$= 0$ otherwise.

- For $E > V_0$, we have positive kinetic energy at all x, and hence its oscillatory everywhere with less probability of the particle to be in the finite potential region. The solutions are bunch of plane wave like solutions, called scattering solutions. We will not consider this case any further.
- For $0 < E < V_0$, we have three regions I, II, III as shown in figure. The motivation of this problem is not to study eigenenergy, normalizability of eigenstates etc, but to demonstrate the quantum tunneling between region I & III, via a potential barrier which classically forbid tunneling of classical particle with -ve K.E.

- The Schrödinger equation in three regions are:

$$\underline{I, III}: \quad \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x) \quad -(1)$$

where $k^2 = \frac{2mE}{\hbar^2} \Rightarrow E = \frac{\hbar^2 k^2}{2m}$.

II : $$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E-V_0)\,\psi(x).$$

$$= -k'^2\psi(x) \quad \text{where } k'^2 = \frac{2m(E-V_0)}{\hbar^2} < 0$$

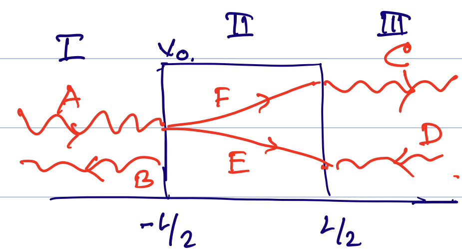
since $E < V_0$.

Therefore, k' is imaginary.

We define $\boxed{k' = i\,k.}$ where $\boxed{k = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}} > 0.$ —(2)

- The solutions of the above two Schrödinger equations are easily obtained as

$$\left.\begin{aligned} \text{I}:&\quad \psi_I(x) = A\,e^{ikx} + B\,e^{-ikx}, \quad \text{for } x < -L/2 \\ \text{III}:&\quad \psi_{III}(x) = C\,e^{ikx} + D\,e^{-ikx}, \quad \text{for } x > L/2. \\ \text{II}:&\quad \psi_{II}(x) = E\,e^{-kx} + F\,e^{kx}, \quad \text{for } -\tfrac{L}{2} < x < L/2 \end{aligned}\right\} \text{—(3)}$$



The interpretation of these solutions are as follows. In region one, we have an incident plane wave of amplitude $|A|$, and a reflected plane wave from the barrier at $x=-L/2$ with amplitude $|B|$. The plane wave however becomes decaying/growing solution inside the barrier with corresponding amplitudes $|E|$ & $|F|$, respectively. Mostly it will decay, with $|E| \gg |F|$. Then, the particle/wave will transmit through the other wall at $x = L/2$ and become again a plane wave with amplitude $|C|$ and some part of it will be incoming in region III with amplitude |D|.

- This problem starts looking similar to the case of a propagating wave is being hit on a transparent (glass) plane and we are asking how much (light) wave pass through the plate and how much is being reflected (& absorption?) In fact, this is indeed the case for the particle's wave nature, and the potential energy V_0 stands for the transparency of the plate. Thus quantum particle can tunnel through a potential barrier, while a classical particle cannot due to negative K.E.

- Our focus here will be to study an incident particle from region I with amplitude |A|, how much it transmit to the region III, is |C| = ? In the classical limit |C| = 0. But quantum mechanics allows tunneling with negative K.E. Its clear that the tunneling probability depends on K, which measures the amplitude of K.E. and the width of the barrier. In fact, the parameter K has the dimension of inverse length $[K] = [L^{-1}]$ and it roughly measures the decay length of the wave. In other words it roughly measures how far the wave can travels before it ceases to exists, ie, how far the wave can tunnel for a given negative K.E.

- Clearly, a rough length scale for the tunneling to occur is when the decay length κ^{-1} is smaller than the width of the barrier i.e.

$$\kappa^{-1} < L .$$

$$\text{or, } \quad \frac{\hbar}{\sqrt{2m(V_0-E)}} < L.$$

$$\Rightarrow \quad \frac{2m(V_0-E)L^2}{\hbar^2} > 1$$

This suggests even for a particle of mass 'm' with $E=0$, it can tunnel a distance of L of potential barrier V_0 if

$$\boxed{\underbrace{\frac{2m V_0 L^2}{\hbar^2}}_{\text{"opacity"}} > 1} \quad \text{---(4)}$$

This dimensionless quantity $\frac{2mV_0L^2}{\hbar^2}$ is called "opacity" or inverse "transparancy".

- This tunneling is happening because of the quantum nature of the particle, i.e. due to having an uncertainty in the value of its position and momentum. Because of this uncertainty in position Δx, there is a probability of finding the particle about Δx around its mean position. This means the wave function is spread atleast by this amount of Δx. This uncertainty in position is the cause of the tunneling and clearly if $\Delta x < L$, then there is a finite probability of finding the particle on the other side of the barrier. The uncertainty Δx depends on the barrier height V_0. In fact the decay length k^{-1} is the measure of this uncertainty. To see that, we start with $\Delta x \sim \hbar / \Delta p$. Now, the momentum uncertainty $\Delta p \sim \sqrt{\langle p^2 \rangle} \sim \sqrt{2m(K.E.)} \sim \sqrt{2m(V_0 - E)}$.

So, we get $\boxed{\Delta x = \Delta p / \hbar \sim \sqrt{\frac{2m(V_0-E)}{\hbar^2}} \sim k}$ [from eq(2)].

- Associated with the decay length, there is then a decay time $\tau \sim \Delta x / v \sim \frac{1}{kv}$, where $v = \frac{\hbar k}{m}$ is the phase velocity (group velocity) of the particle. We get

$$\tau \sim \frac{1}{kv} = \frac{m}{k \hbar k} = \frac{m}{\hbar} \sqrt{\frac{\hbar^2}{2m(V_0-E)}} \sqrt{\frac{\hbar^2}{2mE}}$$

$$\sim \frac{\hbar}{\Delta E}, \text{ where } \Delta E \sim \sqrt{\langle E^2 \rangle}$$

• Let us now return to eq (3) and obtain the coefficients A,...,F by using boundary conditions.

The wave function and its 1st derivative must be continuous at all positions.

- At $x = -L/2$: $\psi_I(-L/2) = \psi_{II}(-L/2)$. --- (5a)

$$\left.\frac{d\psi_I}{dx}\right|_{x=-L/2} = \left.\frac{d\psi_{II}}{dx}\right|_{x=-L/2} \quad \text{--- (5b)}$$

$$(5a) \Rightarrow A e^{-ikL/2} + B e^{ikL/2} = E e^{\kappa L/2} + F e^{-\kappa L/2}$$

$$(5b) \Rightarrow A e^{-ikL/2} - B e^{ikL/2} = \frac{-\kappa}{ik}\left(E e^{\kappa L/2} - F e^{-\kappa L/2}\right).$$

Define a complex quantity $q = \frac{1}{2}(k + i\kappa)$. Then we have

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{k}\begin{pmatrix} q\, e^{i q^* L} & q^* e^{i q L} \\ q^* e^{-i q L} & q\, e^{-i q^* L} \end{pmatrix}\begin{pmatrix} E \\ F \end{pmatrix} \quad \text{— (6)}$$

Similarly, at $x = L/2$, we match ψ_{II} & ψ_{III} and their derivatives

$$\begin{pmatrix} E \\ F \end{pmatrix} = \frac{i}{\kappa}\begin{pmatrix} -q\, e^{i q^* L} & q^* e^{-i q L} \\ q^* e^{i q L} & -q\, e^{-i q^* L} \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix} \quad \text{— (7)}$$

- By combining eqs (6), (7), we can get a relation between A, B & C, D, which will tell us how much wave function pass through the barrier and how much is reflected back. So, we get

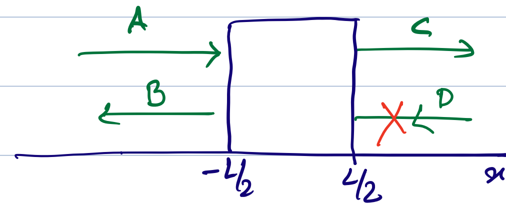
$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix} \quad \text{— (8)}$$

where $M_{11} = M_{22}^* = \left(\cosh \kappa L + \frac{i\varepsilon}{2}\sinh \kappa L\right) e^{ikL}$

$M_{12} = M_{21}^* = \frac{i\eta}{2}\sinh \kappa L$.

and $\varepsilon = \frac{\kappa}{k} - \frac{k}{\kappa}$; $\eta = \frac{\kappa}{k} + \frac{k}{\kappa}$, $\Rightarrow \eta^2 - \varepsilon^2 = 4$.

A, B are the incident and reflected wave's amplitudes at the $x = -L/2$ wall, whereas C, D are the transmitted and reflected wave amplitudes at the $x = L/2$ wall.



We will assume that there is incident wave from the right, i.e. $D = 0$. Then we get.

$$\frac{C}{A} = \frac{e^{-ikL}}{\cosh \kappa L + i\frac{\varepsilon}{2}\sinh \kappa L} \quad \text{---} (9)$$

Then the transmission coefficient is defined as

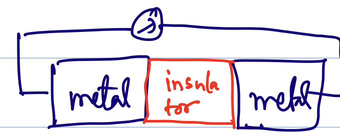
$$T = \frac{|C|^2}{|A|^2} \quad \text{----} (10).$$

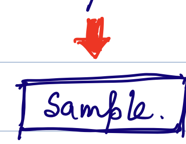
[H.W.: Compute the reflection coefficient at the $x = -L/2$ wall, defined as $R = \frac{B}{A}$ and show that $|R|^2 + |T|^2 = 1$]

$$T = \left[1 + \frac{V_0^2 \sinh^2(\kappa L)}{4E(V_0 - E)}\right]^{-1} \quad \text{---} (11).$$

This is the striking feature of quantum mechanics / wave nature that the particle can <u>tunnel</u> or <u>transmit</u> through a potential barrier.

Its like if we put two metals where electrons are free, and sandwich between them an insulator, then the electron can tunnel between them. If we connect the two metals with an ampmeter, we will be able to measure a finite (usually very small) current. The current density that will be transmitted is $J_t = v|C|^2$ while the current that will be reflected back is $J_r = v(|A|^2 - |B|^2)$, where $v = \hbar k/m$ is the phase velocity. This is the mechanism used in the experiment, called Scanning Tunneling Microscopy, where a metallic tip is scanned slightly above a metallic sample, but the tip is not touched with the sample, causing a potential barrier between the metallic tip and the sample.





(Typically, the average current will be zero, and one needs to provide some bias voltage to give the extra K.E., i.e., increase E close to V_0.)

- This is obvious that as $E \to 0$, the transmission $T \to 0$, and T monotonically increases with E. As $E \to V_0$, $k \to 0$, the transmission coefficient becomes

$$T \to \lim_{E \to V_0} \left(1 + \frac{2mV_0L^2}{\hbar^2}\right)^{-1} \quad \cdots (12)$$

This dimensionless quantity $\boxed{\frac{2mV_0L^2}{\hbar^2}}$ was defined above, called the "opacity" or inverse "transparency" of the barrier.

(D1) In the limit of high (large V_0) and wide (large L), barrier, where the opacity is high, we have $\kappa L >> 1$ and $2\sinh \kappa L \approx 2\cosh \kappa L \approx e^{\kappa L}$ and we obtain

$$T \approx 16 e^{-\kappa L}\left(\frac{k\kappa}{k^2+\kappa^2}\right)^2$$

$$= \frac{16 E(E-V_0)}{V_0^2} e^{-\kappa L} \rightarrow \text{very small.} \quad \text{--- (11).}$$

This formula is often used in Scanning Tunneling Microscopy experiment to fit the data. So, the tunneling is also suppressed exponentially with the length scale of κ^{-1} as the wave function does.

(D2) In another limit of high (large V_0) but narrow (small L) barrier, ie, higher transparency, $\kappa L << 1$ and we have $\sinh \kappa L \approx \kappa L$

$$T \approx \left[1 + \frac{V_0^2 (\kappa L)^2}{4E(V_0-E)}\right]^{-1} = \frac{E}{E + \frac{mV_0^2 L^2}{2\hbar^2}} \quad \text{---(13)}$$

So, there is small but finite tunneling for $E < V_0$.

(D3) Delta Function Potential :

We now think of shrinking the width of the above potential barrier $L \to 0$ and simultaneously we take $V_0 \to \infty$ such that at the product $V_0 L$, which is the area under the potential barrier, remains finite. Lets call this area as $g = V_0 L$. In this limit, the above narrow potential barrier is denoted by a δ-function:

$$V(x) = \lim_{\substack{L \to 0 \\ V_0 \to \infty}} V_0 L = g\,\delta(x) \quad --- (14).$$

Although a dirac delta function is not a function in the usual sense, its integral represents a valid quantity. Such δ-function potentials arise as impurity / disorder scatterers in solid state metals in which the electrons are free but we are asking how do they scatter off from point defects or impurity atoms, etc. Think of a 1D metallic wire. There are defects / impurities in system. If electrons were classical particles, then they would have scattered back from impurities and we would have never obtain any current. But thanks to the quantum nature of electrons, we have finite tunneling of electrons from such narrow potential barrier / delta functions and we obtain finite current.

For the delta function potential, the condition $\kappa L \ll 1$ is still obeyed. Therefore, the transmission coefficient is given by eq (13):

$$T = \frac{E}{E + \frac{mg^2}{2\hbar^2}} \quad \text{--- (15).}$$

The current density $J = v|C|^2 = v|A|^2 T$ remains finite.
$= v(|A|^2 - |B|^2)$

[H.W. Solve the delta function potential problem exactly as we did for the negative δ-fn potential.]

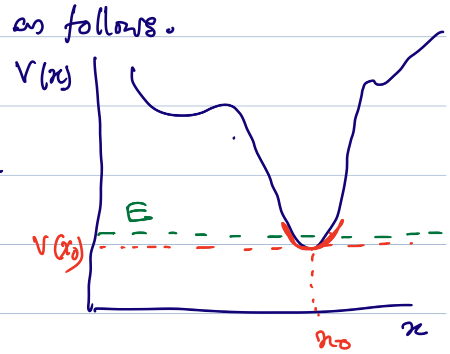
(D4) (H.W.) Solve for the case when $E > V_0$.

E. Simple Harmonic Oscillator :

So far we have only considered constant potentials, confined in a particular region. We will now consider a position-dependent potential $V(x)$. Unfortunately, there are not many potentials that we can solve exactly, and only handful of potential that has exact solutions. For example, simple harmonics oscillator, single particle in a Coulomb potential, charge particle in a magnetic field. We will solve the first two problems in this course, while the last can be solved using the tricks learned in the first problem and will be taught in other courses.

Any continuous potential $V(x)$ at a minimum can be approximated by a Harmonic oscillator as follows.

We can Taylor expand the potential near the minimum for $|x-x_0|<1$ range as

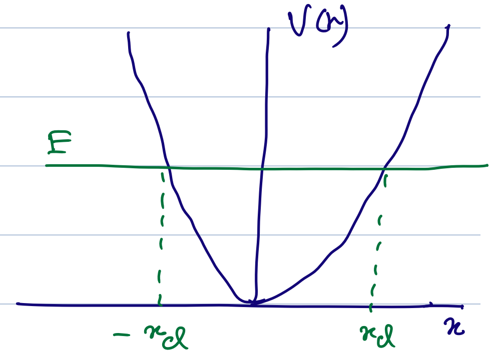


$$V(x) = V(x_0) + \underbrace{\frac{dV}{dx}\bigg|_{x_0}}_{=0}(x-x_0) + \frac{d^2V}{dx^2}\bigg|_{x_0}(x-x_0)^2 + \mathcal{O}\left((x-x_0)^3\right)$$

At the minima, $\frac{dV}{dx}=0$. $V(x_0)$ gives an overall shift to the potential, which eventually shifts all the energy values by a constant value. This shift does not change the overall result and does not appear at the wave function. This is called the zero point energy. So, without loosing generality, we set $V(x_0) = 0$. We also shift $x_0 = 0$ by just a simple shift of reference frame. Finally we define $\left.\frac{d^2V}{dx^2}\right|_{x_0} = \frac{1}{2}k$ where 'k' gives the spring constant. Then we have the simple Harmonic oscillator potential

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

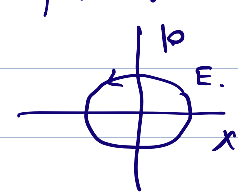
This is a good approximation to the potential as long as the energy E of the system is close to $V(x_0)$, such that the classical turning points $|x_{cl} - x_0| < 1$. The potential in eq(1) is again plotted here. We will no longer concern ourselves with the limit on x and just solve eq(1) as a general potential given to us.



- The classical energy is

$$E = \frac{p^2}{2m} + \frac{1}{2}kx^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 \quad \text{--}(2)$$

where we define a frequency $\omega = \sqrt{k/m}$. This gives an elliptical constant energy contour on the phase phase, but the particle can take any continuous energy. This is the motion of a particle attached to a string which then oscillates around its



equilibrium position, which we set to be at $x=0$. We have also studied many particles attached with each other with springs and then we have seen that there are normal (resonance) modes of vibrations in which all particles vibrate together.

- Atoms in solid can also be modelled by collection of small particles of $\AA$ size, attached with each other via a spring in a periodic manner. Their collective vibrations give similar normal modes ω, but because the atoms are small in size and their distances are in the $\AA$ scales, their vibrations exhibit quantum mechanical nature. Then these vibrational waves have particle dual nature, which are called phonon.

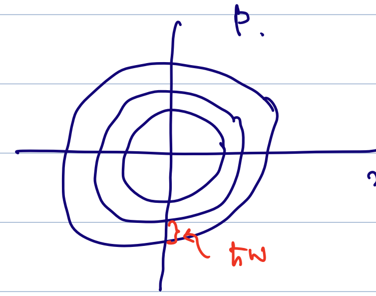
- Here we are only interested in one atom's vibrations. To go from classical to quantum mechanics we need to make x, p as operator, which do not commute anymore.

$$H\psi = \left(\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2\right)\psi$$

$$= \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right)\psi \quad \cdots (3)$$

with $[x, p_x] = i\hbar$. $\quad$ -- (4).

So, that $\Delta x \Delta p \geq \hbar$. We will see that only discrete set of energy contours will now be allowed (ie, only those solutions are normalizable and physically acceptable). These discrete energy contours are separated in units of $\hbar\omega$, as we can anticipate from our introductory lectures, because the phase space is discretized due to uncertainty principle, and the smallest area possible is $\sim h$. So, all the energy contours have to be separated in units of h, and ω comes on ride, both due to dimensional reason and also to incorporate the information about the potential. According to correspondence principle, as $h \to 0$ we should get the classical result, which we indeed get.



We can first try to estimate the lowest possible energy which has to be $\sim \hbar\omega$, occupying the lowest possible area of the phase space, from the uncertainty principle. In all the previous examples, there was a clear length scale in the problem and we said the maximum uncertainty in position is that length scale. In the present case, the potential is growing to infinity and there is no obvious length scale in the problem (If we fix the total energy E, then there is a length scale, ie, the distance between the classical turning points where the kinetic energy goes to zero. Because the wave function must decay outside the classical turning point due to negative K.E., so this length scale can justify a maximum uncertainty in position. You will check yourselve that whether the result below is reproducible or not with this lengthscale. Now we will not assume any fixed energy, and try to obtain the lowest possible energy).

To estimate the uncertainty in x & p, we need to have some idea of how the ground state should look like. First thing we notice from eq(9) is that the Hamiltonian is invariant under $x \to -x$, i.e., its eigenstates have definite parity. Now, the ground state energy is when the particle spends most time at the potential minimum. Therefore, the probability density $\rho(x)$ has a maximum at the potential minimum $x = 0$, and has one extremum, because the ground state energy is something which have the largest spread of its wavepacket. So, the ground state wave function is even under parity. With this information, we can now estimate Δx & Δp: $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$, and so on.

$$\langle x \rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x)\, \hat{x}\, \psi(x) = 0$$

because this this is an odd integral.

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x)\, \hat{x}^2\, \psi(x) \neq 0$$

So, $\Delta x \sim \sqrt{\langle x^2 \rangle}$. Similarly $\langle \hat{p} \rangle$ should also be zero, because otherwise the particle will get out of the spring if it a finite average momentum to be finite. Hence $\Delta p = \sqrt{\langle p^2 \rangle}$. Then the expectation value of the Hamiltonian, which gives us the energy is

$$E = \langle \hat{H} \rangle = \frac{\langle \hat{p}^2 \rangle}{2m} + \frac{1}{2} m \omega^2 \langle x^2 \rangle$$

$$= \frac{1}{2m} (\Delta p)^2 + \frac{1}{2} m \omega^2 (\Delta x)^2 \quad \text{--(4)}.$$

Interestingly, the average energy is determined by the spread in position & momentum. But both Δx & Δp are in the numerator and one could expect the energy is minimized when both $\Delta x \to 0$, $\Delta p \to 0$. But that opposite to what we expect from the uncertainly principle that if $\Delta x \to 0$, then $\Delta p \to \infty$ and vice versa. This would then rather maximize the energy. So, the system will make a compromize between them. We have said that the ground state is obtained when $\Delta p \Delta x \sim \hbar/2$. So we substitute $\Delta p \sim \hbar / \Delta x$ in eq (4),

$$E = \frac{1}{2m} \frac{\hbar^2}{4 (\Delta x)^2} + \frac{1}{2} m \omega^2 (\Delta x)^2.$$

Then we minimize E with respect to Δx.

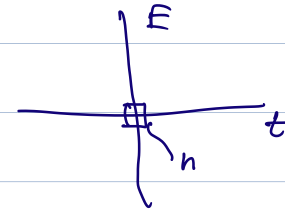
$$\frac{dE}{d(\Delta x)} = \frac{1}{2m} \frac{\hbar^2}{4 (\Delta x)^3} (-2) + m \omega^2 \Delta x. = 0.$$

$$\Rightarrow \quad (\Delta x)^4 = \frac{\hbar^2}{4 m^2 \omega^2}. \quad \text{---(5)}$$

So, we get $\quad E_{\text{ground state}} = \frac{1}{2m}\,\frac{\hbar^2\, 2m\omega}{4\,\hbar} + \frac{1}{2} m\,\omega^2 \cdot \frac{\hbar}{2 m \omega}$.

$$= \frac{1}{2}\hbar\omega \quad . \qquad \text{--(6)}.$$

This is consistent with the smallest phase space area in both position & momentum, as well as in E vs t where $\omega = 2\pi/T$ is the angular frequency and T is the time period. Therefore, the ground state energy is obtained by the time period it takes to complete a single rotation in the smallest phase space area. One may ask will the next energy level be obtained



by the time it takes to complete two rotations? This sometimes works but not always. The reason being, this sort of quantization via phase space volume is the Bohr-Sommerfeld quantization procedure which we categories as old quantum theory. It turns out that not all the integer multiple solutions of $n\hbar\omega = nh/T$ is a normalizable, and/or orthogonal solutions of the Schrödinger equations. That what we have seen in other examples where energy quantizations are obtained in units of n^2, $1/n^2$, etc. Therefore, according to new quantum theory, the normalizability and other boundary conditions puts constraint on the possible solutions and that quantizes the energy eigenvalues. We will see it again for the simple Harmonic oscillator.

- From eq (5), we now have a length scale, as the optimum uncertainty of the ground state wave function. We denote it as κ^{-1}, defined by

$$\kappa^{-1} = \sqrt{2}\,\Delta x = \sqrt{\frac{\hbar}{m\omega}} \quad \text{--- (6).}$$

(Notice that a factor of $\sqrt{2}$ is added just for future convenience).

Is this same as the distance between the two classical turning points x_{cl} ? Its defined by the distances where $E = \frac{1}{2}kx_{cl}^2$. ie, when momentum vanishes. $x_{cl} = \sqrt{\frac{2E}{k}} = \sqrt{\frac{\hbar\omega}{k}}$ $= \sqrt{\frac{\hbar}{m\omega}} = \kappa^{-1}$, where we have substituted $E = \frac{1}{2}\hbar\omega$ & $\omega = \sqrt{\frac{k}{m}}$. So its indeed the classical turning point that determines the maximum uncertainty in position.

(*) Interestingly, we can solve the Schrödinger equation exactly as a differential equation solution.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2\psi = E\psi \qquad -(7)$$

- One thing we notice is that the potential keeps growing forever. Therefore, whatever the energy is, there is a classical turning point and the wavefunction will decay outside the classical turning point. The decay length is $\alpha = k^{-1} = \sqrt{\frac{\hbar}{m\omega}}$. Therefore, there will always be bound state or localized state in this system. From all the knowledge so far, we expect the wave function should decay as $e^{-k|x|}$ in the asymptotic limit of $x \to \pm\infty$. We will however see a slightly different form, i.e., a Gaussian form $e^{-k^2x^2}$ as $x \to \pm\infty$. This function also has the variance k^{-1}. Inside the classical turning point, the kinetic energy is position, and hence we expect oscillatory solutions (wave packets) with quantized wavelengths.

- Before we plunged into solving it, we will first try to simplify the look of the above differential equation by cleaning it up be redefining the position variable in terms of a dimensionless variable u:

$$u = kx = \sqrt{\frac{m\omega}{\hbar}}\,x \qquad \cdots (8).$$

[This sort of choice of dimensionless variable choice is very useful in physics for both to make the equations look simpler, as well as to be able to put it in a computer. But if we want to solve eq(7), its too annoying to put the values of $\hbar \sim 10^{-26}$, $m \sim 10^{-31}$ etc. In fact in most cases, these numbers are even smaller than the smallest numbers any computer can handle. Therefore, choosing a dimensionless variable always gaurantee to make it solvable. For that purpose, we have one problem, i.e. to find a length scale which can hide all the unnecessary variables. Luckily we have a length scale in our problem for a given energy, i.e. k^{-1}.]

Substituting $x = u/k$ in eq(7), we get

$$-\frac{\hbar^2 k^2}{2m}\frac{d^2\psi(u)}{du^2} + \frac{1}{2}\frac{m\omega^2}{k^2}u^2\psi(u) = E\psi(u).$$

Next we substitute $k^{-1} = \sqrt{\frac{\hbar}{m\omega}}$, which gives.

$$-\frac{\hbar\omega}{2}\frac{d^2\psi}{du^2} + \frac{1}{2}\hbar\omega u^2\psi = E\psi$$

$$\Rightarrow \frac{d^2\psi}{du^2} - u^2\psi = -\frac{2E}{\hbar\omega}\psi = -N\psi$$

where $N = \frac{2E}{\hbar\omega}$ a dimensional number. We call it

N, but right now there is no constraint on the possible values of N. This form $E = \frac{\hbar\omega}{2} N$ however does indicate how the energy eigenvalues are going to look like. The boundary conditions will put constraints on the allowed values of n and hence we will obtain the quantization condition.

So, the differential eq we have is

$$\boxed{\frac{d^2\psi}{du^2} = (u^2 - N)\,\psi} \quad \text{---}(9)$$

- Usually, we solve differential equations by series method, which gives some finite/infinite series solution in powers of u. Then as u increases, many of these series diverges and we have a radius of convergence, i.e. some limits on the maximum value of u upto which the series is defined. Here we cannot put such sharp cutoff on u since the potential is monotonically growing in x. We hope there is also exponential part related above the classical turning point which decays faster than the growing power series, then the wavefunction will be normalizable.

So we first study the asymptotic behavior, $u \to \pm\infty$. Since 'N' is a dimensionless constant, it remains finite as $u \to \pm\infty$, so, the differential equation can be written as

$$\frac{d^2\psi}{du^2} \cong u^2 \psi \quad \text{---}(10)$$

This does not have a power law solution because L.H.S decreases two powers of u while R.H.S increases two powers. On the otherhand a function of the form $e^{\pm u^2}$ will work because the 2nd order differential term on the L.H.S have to generate two powers of u which exponential of this form can generate. So, we take an ansatz as the general solution:

$$\psi(u) = f(u)\, e^{-u^2/2} \quad --- (11)$$

We only consider $e^{-u^2/2}$ because that's the solution which will be normalizable. We do expect that $f(u)$ will be a polynomial. Substituting eq (11) in (10), we get

$$\frac{d^2f}{du^2} - 2u\frac{df}{du} + (N-1)f = 0 \quad --- (12).$$

This is actually a well known differential equation (Hermite's PDE)

Its solutions are well known and studied in details in the Math Phys Course. Here we'll focus more on the solution's physical properties and origin of quantization.

First thing we notice is that the original Schrödinger equation is invariant under inversion $x \to -x$. So, the solutions must have definite parity, i.e. they are even & odd under $x \to -x$. Now, in eq (11) $e^{-u^2/2}$ is always even under $u \to -u$. Therefore, $f(u)$ must be even & odd also under parity. This is also clear from the invariance of the Hermite equation under parity $u \to -u$.

- We solve it in the standard series solution method by assuming

$$f(u) = \sum_{j=0}^{\infty} a_j u^j \quad \text{---(13)}.$$

where j are positive integers, because for negative integer, f(u) will have singularity at u=0 which we don't want. We substitute eq (13) in (12) and collect for u^j th term as

$$\sum_{j=0}^{\infty} \left[(j+2)(j+1) a_{j+2} - (2j+1-N) a_j \right] u^j = 0 \quad \text{-(14)}$$

Now since all u^j terms are linearly independent, therefore, if the sum of a series of linearly independent function goes to zero, then every coefficient must vanish. This gives us the recursion relation as

$$\boxed{a_{j+2} = \frac{2j+1-N}{(j+2)(j+1)} a_j} \quad \text{--- (15)}.$$

- We notice in this recursion relation that because it skips one coefficient in between, we need to set two initial values a_0 and a_1 and then every other terms are determined. This is not a problem because Schrödinger eq is 2nd order and we always need to boundary conditions.

- We also observe that because only even and odd parity solutions are allowed, therefore in each wave function either all even terms or all odd terms will contribute, but both will not contribute simultaneously. In other words when $a_0 \neq 0$, $a_1 = 0$ and we have even solutions, f_{even} and when $a_0 = 0$, $a_1 \neq 0$ we have odd solutions f_{odd}. Then essentially we have only one free parameter, a_0 or a_1 which can be determined by the normalization condition.

- ☹ But there is still a serious problem with the general solutions. The infinite series $f(u)$ does not diverge slower than the $e^{-u^2/2}$ term converge. We can check the convergence rate by looking at the ratio between a_{j+2} and a_j in the limit $j \to \infty$ which gives

$$\frac{u^{j+2}}{u^j}\frac{a_{j+2}}{a_j} \simeq \frac{2j}{j(j+3)} u^2 \approx \frac{2}{j+3} u^2$$

So, the coefficients decrease as $1/j$, but we have the u^2 term too. Lets also check how $e^{-u^2/2}$ term converges.

$$e^{-u^2/2} = \sum_{k=0}^{\infty} \frac{1}{k!}\left(-\frac{u^2}{2}\right)^k$$

$$= \sum_{k=0}^{\infty} \frac{1}{k!}\left(-\frac{1}{2}\right)^k u^{2k}.$$

We define $2k = j$ where j takes even integer.

$$= \sum_{j=0,2,\dots} \frac{1}{(j/2)!}\left(-\frac{1}{2}\right)^{j/2} u^j$$

$$= \sum_{j=0,2,\dots} a_j u^j$$

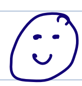
[Same series as $f(u)$].

Then, $\dfrac{a_{k+1} u^{2k+2}}{a_k u^k} = \dfrac{k!\,\left(-\frac{1}{2}\right)^{k+1}}{(k+1)!\,\left(-\frac{1}{2}\right)^{k}} u^2$

$k \to j$

$$= \left(-\frac{1}{2}\right)\frac{1}{j+1}\, u^2$$

Therefore, both $f(u)$ and $e^{-u^2/2}$ diverge and converge, respectively, at the same rate in powers of u^2. Therefore, the series never converges as we integrate from $-\infty$ to ∞, in other words, all solutions are not normazable.

-  There is however a hope. From eq (15), we see that if any of the coefficient a_{j+2} becomes zero at some n^{th} term, then all subsequent higher coeffients also vanishes. Therefore, the series will terminate at a finite n^{th} term. From the recursion relation it clear that it terminates if N takes intergal values such that

$$\boxed{N = 2n+1} \quad \text{---}(16) \quad \text{where } n = 0, 1, 2, \ldots$$

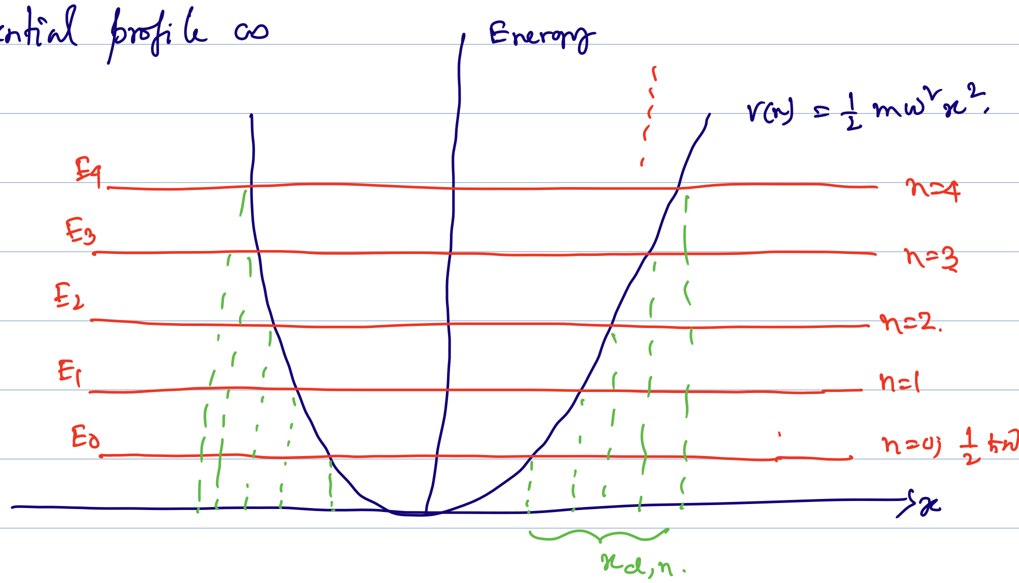
Recall that the energy is defined as

$$\boxed{E = \frac{\hbar\omega}{2} N = \hbar\omega\left(n + \tfrac{1}{2}\right)} \quad -(17).$$

$n = 0, 1, 2, \ldots$

Therefore, the normalizibity requirement of the wave function demands that not all energy eigenvalues are allowed, but only those values which turn out to be integer multiple of $\hbar\omega$ are normalizable and hence provides physical solutions. This is how the quantization of the energy levels arise in modern quantum theory. (The overall shift of $\hbar\omega/2$ is called the zero-point energy and it makes the ground state energy for $n=0$ to be finite.)

We can draw those allowed values of the energy on the potential profile as



We see that every energy levels have different classical turning points and hence the corresponding wavefunction will have different spread or uncertainty. Since the uncertainty is of the order of x_{cl}, it's obvious that the ground state has least uncertainty.

⊛ **Wave functions:** The corresponding wave function for the above eigenvalues are the solution of the following differential equation

$$\frac{d^2 f_n}{du^2} - 2u \frac{df_n}{du} + 2n f_n = 0 \quad \text{--- (18).}$$

This differential equation is called Hermite's differential equation and its solutions are called Hermite polynomials, denoted by $f_n \equiv H_n(u)$. We can actually evaluate all coefficients a_n of f_n from the recursion relation except the constant a_0 for the even values of n and a_1 for odd wavefunctions. This constant can be evaluated by the normalization constant. The Hermite polynomials are actually orthonormalized with the weight factor e^{-u^2} as defined by

$$\int_{-\infty}^{\infty} H_n^*(u)\, H_m(u)\, e^{-u^2}\, du = 2^n n! \sqrt{\pi}\, \delta_{mn}.$$

Then the full wavefunction of the Schrödinger eq is

$$\boxed{\psi_n(u) = N_n\, H_n(u)\, e^{-u^2/2}} \quad \text{where } u = Kx \text{ and } K^{-1} = \sqrt{\frac{\hbar}{m\omega}}.$$

Interestingly, the weight factor e^{-u^2} turns out to be the Gaussian part of the wavefunction so that the wavefunctions are automatically orthonormalized as $\int_{-\infty}^{\infty} \psi_n^*(x)\, \psi_m(x)\, dx = N_n^2 \cdot \delta_{mn}$

where $\quad N_n = \left(\dfrac{K}{2^n n! \sqrt{\pi}}\right)^{1/2}.$

So, we write the full wavefunction as

$$\boxed{\psi_n(x) = \left(\frac{K}{2^n n! \sqrt{\pi}}\right)^{1/2} H_n(Kx)\, e^{-\frac{K^2 x^2}{2}}} \quad \text{--- (19)} \quad \text{where } K^{-1} = \sqrt{\frac{\hbar}{m\omega}}$$

The Hermite polynomials are

$H_0(u) = 1$

$H_1(u) = 2u$

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

$H_3(u) = 8u^2 - 12u.$

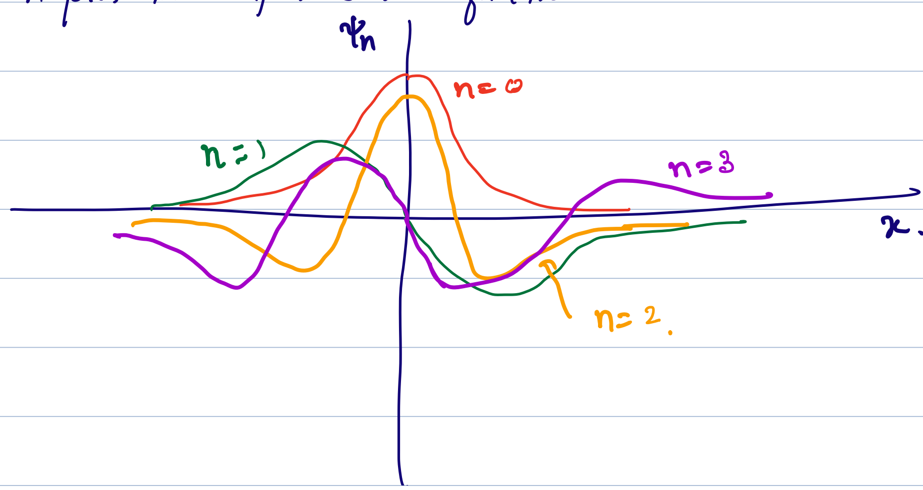
$\vdots$

Alternative Hermite polynomials are even and odd under parity as expected.

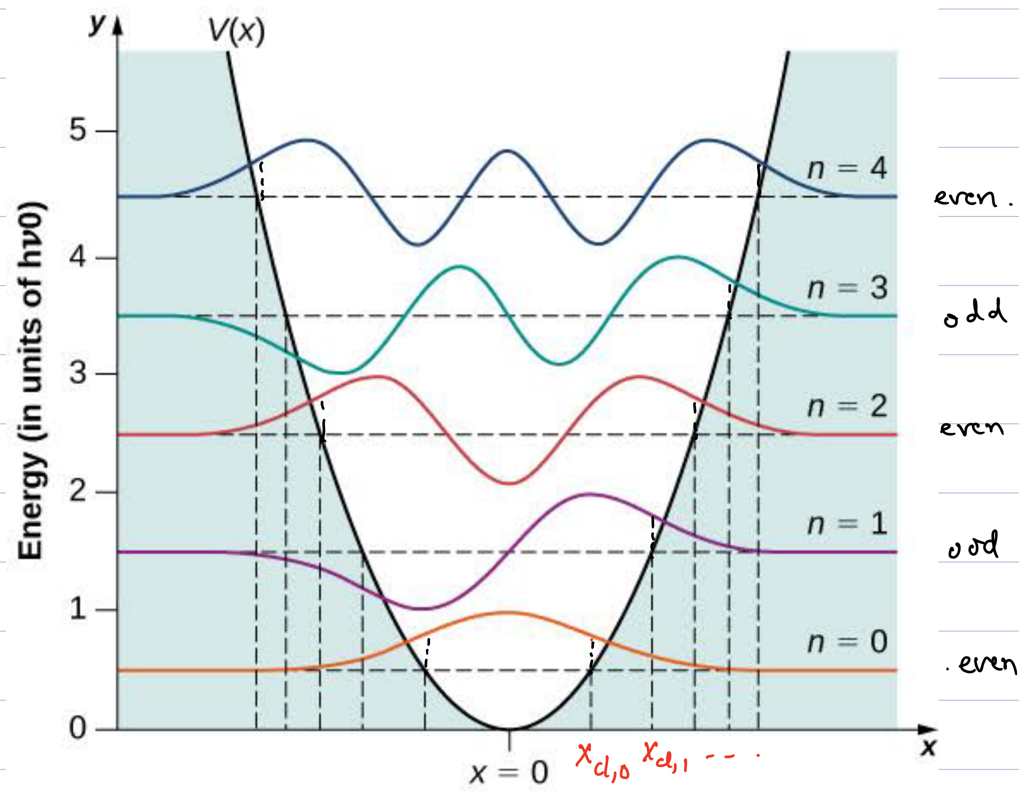
[These Hermite polynomials can alternatively obtained from the Generating function

$$G(u,z) = e^{-z^2 + 2zu} = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(u).\ ]$$

We can plot some of these wave functions:



Alternative wavefunctions are even & odd as expected. Even states have a maximum at $x=0$ and odd states vanishes at $x=0$. They are oscillatory inside the corresponding classical turning point while they decay exponentially outside it. To see that we replot the above eigenfunctions on top of the potential profile and shift each eigenstate vertically up just only for visualization purpose.



As expected, the classical turning point increases with increasing energy levels, and the corresponding wave function is oscillatory inside and decaying outside. The number of extremum increases with increasing energy levels. The spread / uncertainty of the wavefunction for each energy level is still determined by the corresponding x_{cl}.

H.W. 1. (i) Show with explicit calculation that the position uncertainty i.e., the variance in position for each wavefunction $(\Delta x)_n$ matches with its corresponding classical turning point $x_{cl,n}$.

(ii) Also compute the momentum uncertainty in each state. Do you think they can be related to the position uncertainty by the de-Broglie relation? Evaluate $\Delta x \Delta p$ for each level.

(iii) If we have a particle with arbitrary energy E which does not match with any specific eigenenergy of the Harmonic oscillator, but the particle is still attached with a spring. (Think of a vibrating atom which was initially at some eigenstate, then we increase its temperature such that it gains some thermal energy to be liberated from its specific energy level.) How will you express its general state / wavefunction of this system and how will you evaluate its energy now? Explain the physical meaning of all terms.

(iv) We change the potential to $V(x) = \frac{1}{2}kx^2 + \alpha x$. Then evaluate the eigenvalues and eigenfunctions.

(v) Now put an infinite wall at $x=0$ and harmonic potential

$V(x) = \frac{1}{2} k x^2$ only for $x > 0$ and $V = \infty$ for $x < 0$. Sketch the wave function of this potential profile.