Problems on postulates and some simple quantum mechanical potentials

Question 1. Answer the following questions on the postulates of quantum mechanics.

a) What are the fundamental behaviors of the wave function?
b) How can you determine wave function of a quantum particle?
c) What is the meaning of correspondence principle?
d) What is the expectation value and eigenvalue of an operator? When they are the same?
e) What is the meaning of normalization and orthogonalization?
f) What is the meaning of observable? Give two examples?

Answer 1:

a) Fundamental behaviors of the wave function

A wave function $\Psi(x,t)$ must be

Single valued: A single-valued function is function that, for each point in the domain, has a unique value in the range.

Continuous: The function has finite value at any point in the given space.

Differentiable: Derivative of wave function is related to the flow of the particles.

Square integrable: The wave function contains information about where the particle is located, its square being probability density. Therefore $\int_{-\infty}^{\infty}|\Psi(x,t)|^2 dx < \infty$

b) The wave function can be determined by solving Schrödinger equation: $i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(x,y,z)\Psi$, where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ (∇ is Del operator)

c) To every dynamical variable of classical mechanics there corresponds in quantum mechanics a linear, Hermitian operator. When the operators act upon the wavefunction associated with a definite value of that observable yields this value times the wavefunction.

d) Expectation value of an operator is defined as $\langle A\rangle = \int_{-\infty}^{\infty}\psi^* A\psi dx$.When ψ is eigen function of A then expectation value and eigenvalues of the operator is the same.

e) In quantum physics we can calculate probability of finding particle in a given interval [a,b] by using $\int_a^b \psi^*\psi dx$. Normalization means, particle should be exist in the given field and orthogonalization is particle cannot be found in two different state at the same time.

i) An observable is an operator that corresponds to a physical quantity, such as energy, spin, or position, that can be measured.

2. Determine the commutation relation of $[a, a^\dagger] = aa^\dagger - a^\dagger a$, where $a = \frac{1}{\sqrt{2}}\frac{d}{dx} + \frac{1}{\sqrt{2}}x$ and $a^\dagger = -\frac{1}{\sqrt{2}}\frac{d}{dx} + \frac{1}{\sqrt{2}}x$.

Answer 2. a) See lecture notes and class works..

$$[a, a^\dagger] = aa^\dagger - a^\dagger a = \frac{1}{2}\left(\frac{d}{dx} + x\right)\left(-\frac{d}{dx} + x\right) - \frac{1}{2}\left(-\frac{d}{dx} + x\right)\left(\frac{d}{dx} + x\right)$$

$$[a, a^\dagger] = \frac{1}{2}\left(-\frac{d^2}{dx^2} + \frac{d}{dx}x - x\frac{d}{dx} + x^2\right) - \frac{1}{2}\left(-\frac{d^2}{dx^2} - \frac{d}{dx}x + x\frac{d}{dx} + x^2\right)$$

$$[a, a^\dagger] = \left(\frac{d}{dx}x - x\frac{d}{dx}\right) = \left(1 + x\frac{d}{dx} - x\frac{d}{dx}\right) = 1$$

3. A particle is confined to an infinite square well of width a.
   a) Determine wave function and energy.
   b) Normalize wave function.
   c) Show that ground state wave function orthogonal to the 1st excited state wave function.
   d) What is the expectation value of the momentum and energy operator?
   e) Assume that in a measurement wave function of the particle in infinite well is given by $\psi = \sqrt{\frac{1}{a}}\sin\left(\frac{\pi}{a}x\right) + c_1\sin(\frac{3\pi}{a}x)$, calculate c_1, calculate probability of the particles finding each state.

Answer 3. a) We are lucky! Outside the well potential is infinity therefore wavefunction $\psi = 0$. Inside the well potential is zero then Schrödinger equation takes the form: $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$.

Solution of the equation is straightforward: $\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + E\psi = 0 => \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$

Then the solution is $\psi = Asin(kx) + Bcos(kx); where\ k = \sqrt{\frac{2mE}{\hbar^2}}$.

Using boundary conditions $at\ x = 0\ , \psi = 0\ yields\ B = 0$ and other boundary condition

$at\ x = a\ , \psi = 0\ yields\ Asin(ka) = 0\ then\ ka = n\pi; n = 1,2,3$ ...(n=0 is trivial solution)

We can easily obtain$E = \frac{n^2\pi^2\hbar^2}{2ma^2}; E_1 = \frac{\pi^2\hbar^2}{2ma^2}; E_3 = \frac{9\pi^2\hbar^2}{2ma^2}$

b) Normalization is defined as: $\int_0^a \psi^*\psi dx = 1$. Then $\int_0^a Asin(kx)Asin(kx)dx = \mathrm{A}^2\left[\frac{x}{2} - \frac{\sin[2kx]}{4k}\right]_0^a = 1$;

Remember that $k = \frac{n\pi}{a}\ and\ then\ A = \sqrt{\frac{2}{a}}$ is normalization constant.

c)d) See class notes

e) The wave function ψ can be rewritte: $\psi = \frac{1}{\sqrt{2}}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x\right) + c_1\sqrt{\frac{a}{2}}\sqrt{\frac{2}{a}}\sin\left(\frac{3\pi}{a}x\right) = \frac{1}{\sqrt{2}}\psi_1 + c_1\sqrt{\frac{a}{2}}\psi_3$

Normalization condition $\int \psi^*\psi dx = 1$ and orthogonality relation $\int \psi_1^*\psi_3 dx = 0$ yields :

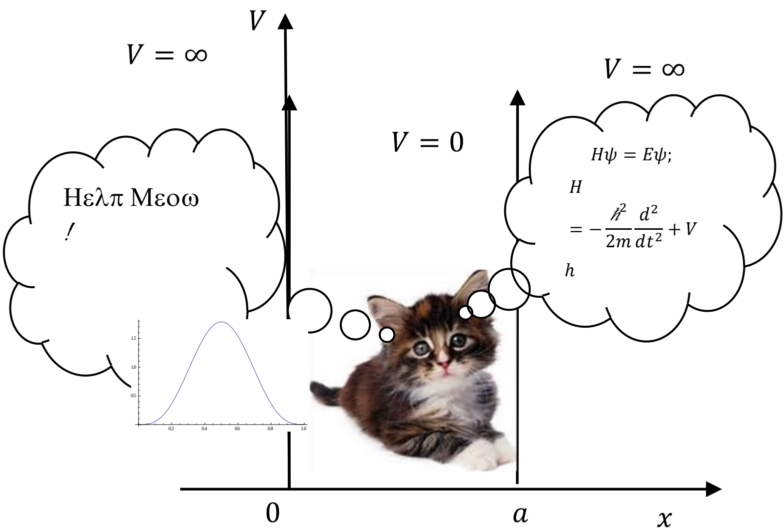
$\left(\frac{1}{\sqrt{2}}\right)^2 + \left(c_1\sqrt{\frac{a}{2}}\right)^2 = 1 => c_1 = \sqrt{\frac{1}{a}}$; Then the wave function $\psi = \frac{1}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{2}}\psi_3$;

Probability of finding of the particles in each state: $\left\{\frac{1}{2}, \frac{1}{2}\right\}$

4. A cat in the infinite square well and informed us initial wave function of the particle:

   $$\Psi(x,0) = Asin^3\left(\frac{\pi x}{a}\right); \quad 0 \le x \le a$$

   a) Determine A.
   b) Find $\Psi(x,t)$.
   c) Calculate $\langle x \rangle$.
   d) Calculate $\langle p^2 \rangle$.
   e) We know that cat can die if average energy of the particle inside the well is greater than $\frac{9\hbar^2\pi^2}{10m}$. Calculate minimum



width of the well, such that cat cannot die.

Answer 4. when we use trigonometric identity: $\sin^3\theta = \frac{3}{4}sin\theta - \frac{1}{4}sin3\theta$, initial wave function takes the form:

$$\Psi(x,0) = A\left(\frac{3}{4}sin\theta - \frac{1}{4}sin3\theta\right)$$

a) Using normalization conditions:

$$1 = \int_0^a |\Psi(x,0)|^2 dx = A^2 \int_0^a \left|\left(\frac{3}{4}\sin\left(\frac{\pi x}{a}\right) - \frac{1}{4}\sin\left(\frac{3\pi x}{a}\right)\right)\right|^2 dx => A = \frac{4}{\sqrt{5a}}.$$

b) Remember, stationary wave function and energy of particle in the infinite well:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right); E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

Then we can write time dependent wavefunction

$$\Psi(x,t) = \frac{1}{\sqrt{10}}\left(3\psi_1(x)e^{-i\frac{E_1}{\hbar}t} - \psi_3(x)e^{-i\frac{E_3}{\hbar}t}\right)$$

c) Absolute square of the wave function is

$$|\Psi(x,t)|^2 = \frac{1}{10}\left(9|\psi_1|^2 + |\psi_3|^2 - 6\psi_1\psi_3\cos\left(\frac{E_1 - E_3}{\hbar}t\right)\right)$$

To calculate expectation value of x:

$$\langle x\rangle = \frac{9}{10}\underbrace{\int_0^a x|\psi_1|^2 dx}_{a/2} + \frac{1}{10}\underbrace{\int_0^a x|\psi_3|^2 dx}_{a/2} - \frac{6}{10}\cos\left(\frac{E_1 - E_3}{\hbar}t\right)\underbrace{\int_0^a x\psi_1\psi_3 dx}_{0} = \frac{a}{2}.$$

d) Momentum operator $p = -i\hbar\frac{d}{dx}$ $then\ p^2 = -\hbar^2\frac{d^2}{dx^2}$:

$$\langle p^2\rangle = \frac{9}{10}\underbrace{\int_0^a \psi_1 p^2\psi_1 dx}_{\frac{9\hbar^2\pi^2}{10a^2}} + \frac{1}{10}\underbrace{\int_0^a \psi_3 p^2\psi_3 dx}_{\frac{9\hbar^2\pi^2}{10a^2}} - \frac{6}{10}\cos\left(\frac{E_1 - E_3}{\hbar}t\right)\underbrace{\int_0^a \psi_1 p^2\psi_3 dx}_{0} = \frac{9\hbar^2\pi^2}{5a^2}.$$

e) Energy $\langle E\rangle = \langle T + V\rangle = \langle T\rangle = \frac{\langle p^2\rangle}{2m} = \frac{9\hbar^2\pi^2}{10ma^2}$

5. a) Write down time dependent and time independent Schrödinger equation.
   b) Show that for time independent potential $V(x)$, Schrödinger equation can be separated in to time and position parts.
   c) Solve the time dependent part of the separated Schrödinger equation.
   d) Write down properties of a valid wave function.
   e) How can you determine physical quantities (observables) of a quantum system by using wave function? Explain.

Answer 5.

a) $i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi$ (Time dependent Schrödinger equation. It is used to calculate energy levels and time dependent wave function of the particles)

$E\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$ (Time independent Schrödinger equation. It is used to calculate energy levels and wave function of the particles)

b) By substituting wave function $\Psi(x,t) = \psi(x)\varphi(t)$ in to Schrödinger equation then applying standart procedure of separation of variable technique we obtain:

$$E\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi \; and \; \frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi.$$

c) Solution of the time part of the equation is straightforward:

$$\frac{\partial\varphi}{\varphi} = -\frac{iE}{\hbar}\partial t$$

integrating both sides we obtain

$$\varphi = e^{-\frac{iE}{\hbar}t}$$

d)e) see class notes.

Hints:

$$\int_0^a \sin\left(\frac{n\pi}{a}x\right)\sin\left(\frac{m\pi}{a}x\right)dx = \begin{cases} \frac{a}{2} & if\ n = m \\ 0 & if\ n \neq m \end{cases}$$

$$\int_0^a \sin\left(\frac{n\pi}{a}x\right)\cos\left(\frac{m\pi}{a}x\right)dx = \begin{cases} 0 & if\ n = m \\ \frac{a(-n + n\cos[m\pi]\cos[n\pi])}{(m^2 - n^2)\pi} & if\ n \neq m \end{cases}$$

$$\int_0^a x\sin^2\left(\frac{n\pi}{a}x\right)dx = \frac{a^2n^2\pi^2}{4n^2\pi^2}$$

$$\int_0^a x^2\sin^2\left(\frac{n\pi}{a}x\right)dx = \frac{1}{12}a^3\left(2 - \frac{3}{n^2\pi^2}\right)$$

$$\sin^3\theta = \frac{1}{4}(3sin\theta - \sin 3\theta); \sin^2\theta = \frac{1}{2}(1 - cos2\theta)$$

$$c = 3\times 10^8\frac{m}{s}; e = -1.6\times 10^{-19}C$$

6. Consider particles incident on a one-dimensional step function potential

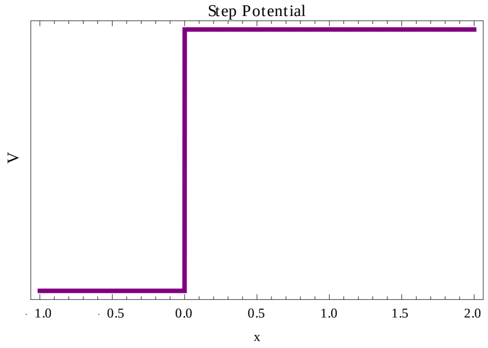
$$V(x) = \begin{cases} 0 & if\ x < 0 \\ V_0 & if\ x > 0 \end{cases}$$

with energy $E > V$.

a) Write down Schrödinger equation fort his system.
b) Determine the wave functions.
c) Calculate the reflection and transmission coefficients.
d) Consider the limits $E \rightarrow V_0$ and $E \rightarrow \infty$.

Answer 6

Step Potential



Consider a particle of mass m and energy $E > 0$ interacting with the simple square barrier:

$$V(x) = \begin{cases} 0 & if\ x < 0 \\ V_0 & if\ x > 0 \end{cases}$$

$$\psi = \begin{cases} e^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{ik'x} & x > 0 \end{cases}$$

Where

$$k = \sqrt{\frac{2mE}{\hbar}};\quad k' = \sqrt{\frac{2m}{\hbar}(E - V_0)}$$

Continuity of the wave function at $x = 0$ give:

$$1 + B = C\,; k(1 - B) = k'C$$

Solution of the equations for B and C:

$$B = \frac{k - k'}{k + k'};\ C = \frac{2k}{k + k'}$$

Reflection and transmission coefficients can be calculated as follows: J is the probability current density.

$$J = \frac{\hbar}{i2m}\left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right)$$

Then

$$J_i = \frac{\hbar}{i2m}(2ik);\ J_r = \frac{\hbar}{i2m}|B|^2(-2ik),\ J_t = \frac{\hbar}{i2m}|C|^2(2ik')$$

Reflection and transmission coefficients

$$R = \frac{|\psi_r|^2}{|\psi_i|^2} = \frac{J_r}{J_i} = |B|^2 = \left(\frac{k - k'}{k + k'}\right)^2$$

$$T = \frac{|\psi_t|^2}{|\psi_i|^2} = \frac{J_t}{J_i} = \frac{k'}{k}|C|^2 = \frac{k'}{k}\left(\frac{2k}{k + k'}\right)^2$$

Where subscripts t, r and i stand for transmission, reflection and incident respectively.
Since the current is a conserved quantity then

$$J_i + J_r = J_t$$

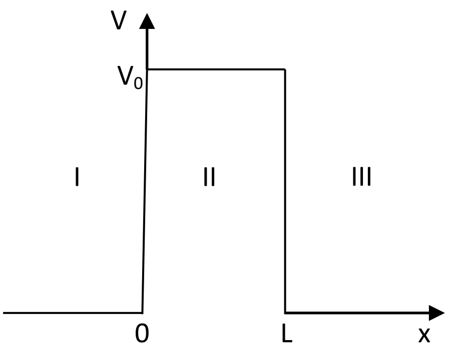
We check that

$$T + R = \left(\frac{k - k'}{k + k'}\right)^2 + \frac{k'}{k}\left(\frac{2k}{k + k'}\right)^2 = 1$$

7. Barrier Problem

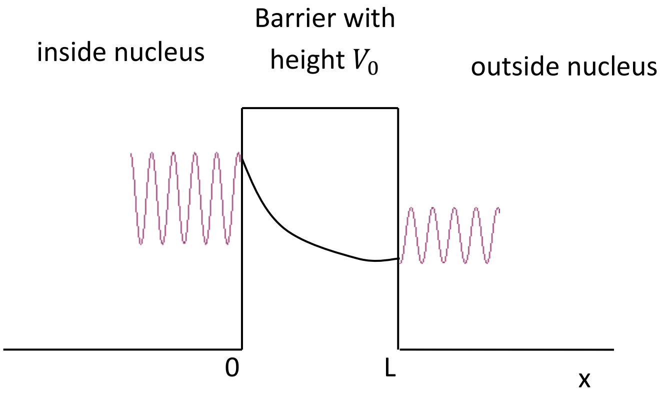
A particle with kinetic energy E strikes a barrier with height $V_0 > E$ and width L as in figure.

a) Write Schrödinger equation for each three region.



b) Solve the Schrödinger equation and obtain wavefunction for each region.

c) The nuclear potential energy can be modelled as a barrier potential as in the figure. Energy of alpha particles within the nucleus less than height of the nuclear potential barrier, but has some chance tunneling through the barrier. For values of $= 1, V_0 = 1\ (units)$, transmission probability is given in the table. If 1000 particle incident on the barrier, what is the number of particle pass through the barrier. Give your answer on the table.



Energy (Unit)	Transmission Probability	#particle pass Through barrier
0.	0.	0
0.1	0.23	230
0.2	0.38	380
0.3	0.49	490
0.4	0.57	570
0.5	0.63	630
0.6	0.68	680
0.7	0.72	720
0.8	0.75	750
0.9	0.78	780

a) Schrödiger equation for the 1st, 2nd and 3th regions are given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} = E\psi_1, \qquad -\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V_0\psi_2 = E\psi_2 \ and \ -\frac{\hbar^2}{2m}\frac{d^2\psi_3}{dx^2} = E\psi_3$$

b) Wave function of the particle is given by

$$\psi_1 = e^{ikx} + Be^{-ikx}$$

$$\psi_2 = Ce^{ik\prime x} + De^{-ik\prime x}$$

$$\psi_3 = Fe^{ikx}$$

8. Consider a normalized state which is given in terms of three orthonormal vectors, $|\phi_1\rangle$, $|\phi_2\rangle$and $|\phi_3\rangle$ as follows:

$$|\psi\rangle = A\,|\phi_1\rangle + \frac{1}{\sqrt{3}}|\phi_2\rangle + \frac{1}{\sqrt{6}}\,|\phi_3\rangle$$

(a) Find the real constant A.

(b) Find the probability of finding the system in $|\phi_1\rangle, |\phi_2\rangle\ and\ |\phi_3\rangle$ using the relations $|\langle\psi|\phi_1\rangle|^2$, $|\langle\psi|\phi_2\rangle|^2\ and\ |\langle\psi|\phi_3\rangle|^2$ respectively.

9. a) What are the energy states of particle in 3D cubic box of side a?

b) Find energy of 6th energy level?

c) What is the degree of degeneracy of 6th energy level?