CHAPTER 2
Schrödinger Equation
Brief Notes and Problems

Brief Notes
As I mentioned before, Schrödinger equation is the fundamental equation of the quantum universe. You can learn more about the solution and application of the Schrödinger equation when you read chapter 2 of Griffiths, Quantum Mechanics and my class notes.

Here I will briefly introduce two topics: Operators and Eigenvalue problems.

Construction of operators using position and momentum operator:
In order to construct quantum mechanical operators, first we write classical observable in terms of momentum and position and then we substitute representation of position and momentum operator.

Representation of momentum operator: \( p_x = -i\hbar \frac{\partial}{\partial x} \); \( p_y = -i\hbar \frac{\partial}{\partial y} \); \( p_z = -i\hbar \frac{\partial}{\partial z} \)

Representation of position operator: \( x, y \text{ and } z \).

Example: Energy equation for the classical Harmonic oscillator is \( E = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 \). Write down Hamiltonian of the oscillator.

Since \( p_x = -i\hbar \frac{\partial}{\partial x} \text{ and } x = x \); then \( E = H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2 \)

Commutator Algebra

Commutation relation of two operator can be defined as:

\[ [A, B] = AB - BA \]

where A and B are operators.

Example. Calculate commutation relation between momentum and position operator.

\[ [p_x, x] = \left[-i\hbar \frac{\partial}{\partial x}, x\right] = \left(-i\hbar \frac{\partial}{\partial x} x\right) - \left(-i\hbar x \frac{\partial}{\partial x}\right) \]

\[ = i\hbar \left(-\frac{\partial}{\partial x} x + x \frac{\partial}{\partial x}\right) \]

We evaluate first term

\[ \left( \frac{\partial}{\partial x} x \right) \psi = \left( x + x \frac{\partial}{\partial x} \right) \psi = x \frac{\partial}{\partial x} \psi \]

Combine the last two equation, we obtain:

\[ [p_x, x] = -i\hbar \]

Angular Momentum operator. Classical definition of the angular momentum is given by

\[ L = r \times p \]
here \( r = x i + y j + z k \) and \( p = p_x i + p_y j + p_z k = -i \hbar \left( \frac{\partial}{\partial x} i + \frac{\partial}{\partial y} j + \frac{\partial}{\partial z} k \right) \)

where \( i, j, k \) are unit vectors and constant with respect to time and coordinate. The cross product yields

\[
L_x = -i \hbar \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right),
\]

\[
L_y = -i \hbar \left( z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right),
\]

\[
L_z = -i \hbar \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right).
\]

**Example.** Consider the operators

\[
a = \sqrt{\frac{m}{2}} \omega x + \frac{ip_x}{\sqrt{2m}}
\]

\[
a^+ = \sqrt{\frac{m}{2}} \omega x - \frac{ip_x}{\sqrt{2m}}
\]

Calculate \( a^+ a \) and find the commutation relation \([a, a^+]\).

Solution:

\[
a^+ a = \left( \sqrt{\frac{m}{2}} \omega x - \frac{ip_x}{\sqrt{2m}} \right) \left( \sqrt{\frac{m}{2}} \omega x + \frac{ip_x}{\sqrt{2m}} \right)
\]

\[
= \frac{m \omega^2}{2} x^2 + \frac{i \omega}{2} p_x - \frac{i \omega}{2} p_x x + \frac{p_x^2}{2m}
\]

Calculating \( \frac{i \omega}{2} p_x - \frac{i \omega}{2} p_x x = \frac{i \omega}{2} (xp_x - p_xx) = \frac{i \omega}{2} (xp_x - (-i \hbar + xp_x)) = -\frac{\hbar \omega}{2} \)

Then

\[
a^+ a = \frac{p_x^2}{2m} + \frac{m \omega^2}{2} x^2 - \frac{\hbar \omega}{2}
\]

Compare the result with harmonic oscillator Hamiltonian!!!!!!

**Eigenvalue equations and expectation values**

It is obvious that when an operator acting on a function maps it on to another function. Let us consider Hamiltonian operator:

\[
H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)
\]

The equation

\[
H \psi = E \psi; \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi = E \psi
\]
is an eigenvalue equation. In the equation $\psi$ is eigenfunction of Hamiltonian $H$ and $E$ is eigenvalues of $H$. If a function eigenfunction of the operator $O$ then expectation values and eigenvalues of the operator $O$ is equal to each others.

**Example:**

Calculate eigenfunction of the momentum operator.

**Solution:** We can write eigenvalue equation: $p_x \phi = k \phi \Rightarrow -i\hbar \frac{d}{dx} \phi = k \phi$

Solution of the differential equation yields:

$$\phi = Ae^{\frac{ik}{\hbar}x}$$

$\phi$ is eigenfunction of the momentum operator.

Example: Is $\phi$ also eigenfunction of Hamiltonian $H$ with a potential $V = \frac{1}{2}m\omega^2x^2$?

Solution: We apply $H$ on $\phi$, then:

$$H\phi = E\phi; \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2\right)Ae^{\frac{ik}{\hbar}x} = EAe^{\frac{ik}{\hbar}x}$$

Then $\frac{k^2}{2m} + \frac{1}{2}m\omega^2x^2 \neq E$. Thus $\phi$ is not eigenfunction of Hamiltonian $H$.

**Heisenberg Uncertainty Principle**

In the previous section we have define uncertainty relation of the operators: if $[A, B] = iC$ then uncertainties in $A$ and $B$ defined as

$$\Delta A^2 = \langle A^2 \rangle - \langle A \rangle^2$$

Obey the relation:

$$\Delta A\Delta B \geq \frac{1}{2} |\langle C \rangle|$$

The uncertainty between momentum and position operator is:

$$[p, x] = i\hbar$$

Then uncertainty

$$\Delta p\Delta x \geq \frac{1}{2} |\langle h \rangle|$$

As it is expected.

**Stationary and Superposition state:**

See class notes….

**Problems**

1. Show that, after separating variables, time dependent Schrödinger equation

$$\frac{i\hbar \partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi$$
takes the form
\[ E\psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi \]

2. Define stationary state.
3. Define ground state.
4. Show that general solution of the Schrödinger equation is the linear combinations of the each separable solutions.

**Solution:**
There is a different wave function for each energy levels, such that:
\[
\Psi_1(x, t) = \psi_1(x) e^{\frac{iE_1}{\hbar}t} \\
\Psi_2(x, t) = \psi_2(x) e^{\frac{iE_2}{\hbar}t} \\
\vdots \\
\Psi_n(x, t) = \psi_n(x) e^{\frac{iE_n}{\hbar}t}
\]

General solution can be constructed as:
\[
\Psi(x, t) = \sum_{n=0}^{\infty} c_n \psi_n(x) e^{\frac{iE_n}{\hbar}t}
\]

To complete the solution substitute the equation into time dependent Schrödinger equation.

**Particle in the infinite well**

5. Consider a particle in a 1-D infinite square well of width \(a\), arranged to the coordinate system as shown in the figure.

\[ V(x) = \begin{cases} 
\infty & \text{if } 0 < x < a \\
0 & \text{if } x = 0, x = a \\
\infty & \text{outside the well}
\end{cases} \]

(a) Verify that \( \psi_n(x) = A_n \sin k_n x + B_n \cos k_n x \) satisfies time independent Schrödinger’s equation for the region inside the well.
(b) Apply the boundary conditions at \( x = 0 \) and \( x = a \), and normalization condition to determine energy and integral constants.
(c) Show that the particle’s energy is
(d) Show that $\psi_n(x)$ is orthogonal.
(e) Calculate expectation values of Hamiltonian operator $H$.
(f) Write down time dependent form of the wave function.

(g) Suppose that wave function of the particle is given by $\psi = \sqrt{\frac{1}{a}} \sin \left( \frac{2\pi}{a} x \right) + c_3 \cos \left( \frac{\pi}{a} x \right)$, calculate $c_1$, calculate probability of the particles finding each state.

6. Schrödinger’s cat in the infinite well. The well include radioactive particles whose wave function described by Schrödinger equation. At an instant if the cat is exposed more than $\frac{\hbar^2}{2ma^2}$ unit energy it may die. The wave function of the particles are measured:

$$\psi = \sqrt{\frac{1}{4a}} \sin \left( \frac{\pi}{a} x \right) + \sqrt{\frac{1}{2a}} \sin \left( \frac{2\pi}{a} x \right) + c_3 \sqrt{\frac{1}{2a}} \sin \left( \frac{3\pi}{a} x \right) + \sqrt{\frac{1}{4a}} \sin \left( \frac{4\pi}{a} x \right)$$

a) Calculate $c_3$, so that $\psi$ is normalized.
b) The cat takes a walk from one state to the other. Is the cat died or alive?

Solution:
a) Using orthogonality and normalization relations:

$$\int_0^a \psi^* \psi \, dx = 1 = \frac{a}{2} \left( \frac{1}{4a} + \frac{1}{2a} + c_3^2 c_3 \frac{1}{2a} + \frac{1}{4a} \right) \implies c_3 = \sqrt{2}$$

b) Let us start by recalling wavefunction and energy of the 1D infinite well:

$$\phi_n = \sqrt{\frac{2}{a}} \sin \left( \frac{n\pi}{a} x \right); \quad E = \frac{n^2 \hbar^2 \pi^2}{2ma^2}$$
Then we can write the measured function:

$$\psi = \frac{1}{2} \sqrt{\frac{1}{2}} \phi_1 + \frac{1}{2} \phi_2 + \sqrt{\frac{1}{2}} \phi_3 + \frac{1}{2} \sqrt{\frac{1}{2}} \phi_4$$

Corresponding energies

$$E_1 = \frac{h^2 \pi^2}{2ma^2}; E_2 = \frac{4h^2 \pi^2}{2ma^2}; E_3 = \frac{9h^2 \pi^2}{2ma^2}; E_4 = \frac{16h^2 \pi^2}{2ma^2}$$

Then we can say that if cat walk through 3th or 4th states then cat can die.

The probability of finding of cat in the first state: $1/8 \times 100 = 12.5\%$

The probability of finding of cat in the second state: $1/4 \times 100 = 25.0\%$

The probability of finding of cat in the third state: $1/2 \times 100 = 50.0\%$

The probability of finding of cat in the fourth state: $1/8 \times 100 = 12.5\%$

Then the probability for cat live: 37.5%; Die 62.5%.

7. (Problem 2.7, Griffiths) A particle in the infinite square well has the initial wave function

$$\Psi(x, 0) = \begin{cases} Ax & 0 \leq x \leq \frac{a}{2} \\ A(a-x) & \frac{a}{2} \leq x \leq a \end{cases}$$

a) Sketch $\Psi(x, 0)$ and determine constant A.

b) Find $\Psi(x, t)$.

c) What is the probability that a measurement of energy would yield the value $E_1$?

d) Find the expectation value of energy.

Solution: a)
b) 

\[
C_n = \sqrt{\frac{2 \cdot 2\sqrt{3}}{a \cdot a \cdot a}} \left[ \int_0^{2a} x \sin \left( \frac{n \pi x}{a} \right) dx + \int_{2a}^{a} (a-x) \sin \left( \frac{n \pi x}{a} \right) dx \right] = \begin{cases} 
0 & \text{n is even} \\
\frac{(n-1)}{2} \cdot \frac{4\sqrt{6}}{(nn)^2} & \text{n is odd}
\end{cases}
\]

Therefore wave function can be written as:

\[
\Psi(x,t) = \frac{4\sqrt{6}}{n\pi^2} \sqrt{2} \sum_{n=1,3,5...}^{\infty} (-1)^{n-1} \frac{1}{n^2} \sin \left( \frac{n \pi x}{a} \right) e^{iE_n t}; \text{where } E_n = \frac{n^2 \pi^2 h^2}{2ma^2}
\]

c) \(P_1 = c_{1}^2 = \frac{16 \pi^6}{\pi^4} = 0.9855\)

d)

\[
\langle H \rangle = \sum_{n=1,3,5}^{\infty} c_{n}^2 E_n = \frac{96 \pi^2 h^2}{\pi^4 2ma^2} \left( \frac{1}{1} + \frac{1}{3^2} + \cdots \right) = \frac{96 \pi^2 h^2}{\pi^4 2ma^2} \left( \frac{\pi^2}{8} \right) = \frac{6h^2}{ma^2}
\]

**Harmonic oscillator**

8. Operator Algebra

a) Determine the commutation relation of \([a, a^\dag]\), where 

\[
a = \frac{1}{\sqrt{2}} \sqrt{\frac{h}{m \omega}} \frac{d}{dx} + \frac{1}{\sqrt{2}} \sqrt{\frac{m \omega}{h}} x
\]

\[
a^\dag = -\frac{1}{\sqrt{2}} \sqrt{\frac{h}{m \omega}} \frac{d}{dx} + \frac{1}{\sqrt{2}} \sqrt{\frac{m \omega}{h}} x.
\]

b) What is the result of \(a \psi_0, \ a^\dag \psi_0, \ a^\dag a \psi_0 \) and \(a a^\dag \psi_0\) where \( \psi_0 = \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} e^{-m \omega x^2/2} \)?

c) Are whether or not \( \psi_0 \) eigenfunction of \( a^\dag, a, a^\dag a, \) and \( a a^\dag \)?

d) Using action of \( a^\dag \) on the ground state wave function \( \psi_0 \) determine first 2 eigenstate of the oscillator as a function of \( x \).

9. Expectation values

Determine expectation values of momentum, position, potential and kinetic energy of the nth state of harmonic oscillator.

10. (Problem 2.10, Griffiths)

a) Construct \( \psi_2(x) \).

b) Sketch \( \psi_0(x), \psi_1(x), \psi_2(x) \).
c) Check the orthogonality of $\psi_0(x), \psi_1(x), \psi_2(x)$.

**Solution**

a) Acting the operator $a^\dagger = -\frac{1}{\sqrt{2}} \sqrt{\frac{\hbar}{m\omega}} \frac{d}{dx} + \frac{1}{\sqrt{2}} \sqrt{\frac{m\omega}{\hbar}} x$ on $\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-m\omega x^2/2\hbar}$ we obtain:

$$\psi_1 = a^\dagger \psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{2m\omega}{\hbar} xe^{-m\omega x^2/2\hbar}$$

$$\psi_2 = \frac{1}{\sqrt{2}} a^\dagger \psi_1 = \frac{1}{\sqrt{2}} \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \left(\frac{2m\omega}{\hbar} x^2 - 1\right) e^{-m\omega x^2/2\hbar}$$

b) Graph of the wave functions:

![Wave Function Graphs](image)

c) Since $\psi_0$ and $\psi_2$ are even and $\psi_1$ is odd, then $\int_{-\infty}^{\infty} \psi_1^* \psi_2 \, dx$ and $\int_{-\infty}^{\infty} \psi_1^* \psi_0 \, dx$ are vanishes. Please check: $\int_{-\infty}^{\infty} \psi_0 \psi_2 \, dx = 0$.

11. (Problem 2.13 Griffiths) A particle in the harmonic oscillator potential starts out in the state

$$\Psi(x, 0) = A(3\psi_0(x) + 4\psi_1(x))$$

a) Find A.

b) Construct $\Psi(x, t)$ and $|\Psi(x, t)|^2$.

c) Find expectation values of $x$ and $p$. Don't get too excited if they oscillate at the classical frequency: What would it have been had I specified $\psi_2(x)$ instead of $\psi_1(x)$? Check that Ehrenfest theorem (eq. 1.38) holds for this wave function. (Ehrenfest theorem: Expectation values obey classical laws)

d) If you measure energy of this particle, what values might you get and with what probabilities?

**Solution**
a) Normalization yields:

$$\int_{-\infty}^{\infty} \Psi^* \Psi \, dx = A^2 \int_{-\infty}^{\infty} (9\psi_0^* \psi_0 + 12\psi_0^* \psi_1 + 12\psi_1^* \psi_0 + 16\psi_1^* \psi_1) \, dx$$

$$= A^2 (9 + 0 + 0 + 16) = 1 \Rightarrow A = \frac{1}{5}.$$  

b) Time dependent wave function:

$$\Psi(x, t) = \frac{1}{5} \left( 3\psi_0(x)e^{-\frac{i\omega t}{2}} + 4\psi_1(x)e^{-\frac{3i\omega t}{2}} \right)$$

$$|\Psi(x, t)|^2 = \frac{1}{25} (9\psi_0^* \psi_0 + 16\psi_1^* \psi_1 + 12(\psi_0^* \psi_1 + \psi_1^* \psi_0)cos\omega t$$

c) Expectation values of x

$$\langle x \rangle = \frac{1}{25} \int_{-\infty}^{\infty} (9\psi_0^* x \psi_0 + 16\psi_1^* x \psi_1 + (\psi_0^* x \psi_1 + \psi_1^* x \psi_0)cos\omega t) \, dx$$

the terms: \( \frac{1}{25} \int_{-\infty}^{\infty} (9\psi_0^* x \psi_0) \, dx = \frac{1}{25} \int_{-\infty}^{\infty} (16\psi_1^* x \psi_1) \, dx = 0 \) then

$$\langle x \rangle = \frac{1}{25} \int_{-\infty}^{\infty} ((\psi_0^* x \psi_1 + \psi_1^* x \psi_0)cos\omega t) \, dx = \frac{24}{25} \sqrt{\frac{\hbar}{2m\omega}} cos\omega t$$

Expectation values of momentum

$$\langle p \rangle = m \frac{d}{dt} \langle x \rangle = \frac{24}{25} \sqrt{\frac{\hbar\omega}{2}} \sin\omega t.$$  

Ehrenfest theorem says: \( \frac{d}{dt} \langle p \rangle = -\langle \frac{\partial V}{\partial x} \rangle \)

$$-\langle \frac{\partial V}{\partial x} \rangle = -m\omega^2(x) = -\frac{24}{25} \sqrt{\frac{\hbar\omega}{2}} \omega cos\omega t$$

$$\frac{d}{dt} \langle p \rangle = -\frac{24}{25} \sqrt{\frac{\hbar\omega}{2}} \omega cos\omega t$$

Ehrenfest theorem holds.

d) \( E_0 = \frac{1}{2} \hbar \omega \) with a probability 9/25 and \( E_1 = \frac{3}{2} \hbar \omega \) with a probability 16/25.
Free Particle

12. Consider a particle moving in one-dimension characterized by the wavefunction 
\[ \Psi(x, t) = e^{i(kx - \omega t)} \] that is obtained from the solution of the Schrödinger equation for free particle. Write expressions for the following quantities:

(a) Show that the parameters are constrained to 
\[ \frac{\hbar^2 k^2}{2m} = \hbar \omega. \]
(b) What is the momentum of the wave? Ans: \( p = \hbar k \).
(c) What is the speed of the wave? Ans: \( v_{\text{quantum}} = \frac{\sqrt{2E}}{2m} = \frac{\hbar k}{2m} \).
(d) What is the classical speed of the wave? \( v_{\text{classical}} = \frac{\sqrt{2E}}{m} = 2v_{\text{quantum}}. \)
(e) Obtain group and phase velocities and compare with classical and quantum velocities.
\[ v_g = \frac{da}{dk}; v_p = \frac{\omega}{k} \] then \( v_{\text{classical}} = v_g \) and \( v_{\text{quantum}} = v_p. \)
(f) Is this wave function normalizable? Why? Ans: A free particle can not exist in a stationary state.

13. A free particle has an initial wavefunction 
\[ \Psi(x, 0) = Ae^{-\alpha|x|} \] where \( A \) and \( \alpha \) are positive real constants.

(a) Normalize \( \Psi(x, 0) \).
(b) Find \( \phi(k) \).
(c) Construct \( \Psi(x, t) \).

Solution

(a) Using the normalization
\[ A^2 \int_{-\infty}^{\infty} e^{-2\alpha x} dx = 2A^2 \int_{0}^{\infty} e^{-2\alpha x} dx = 1 \Rightarrow A = \frac{1}{\sqrt{\alpha}} \]
(b) The function
\[ \phi(k) = \frac{\sqrt{\alpha}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\alpha x} e^{-ikx} dx = \frac{\sqrt{\alpha}}{\sqrt{2\pi}} \frac{2\alpha}{\sqrt{2\pi k^2 + \alpha^2}} \]
(c) The time dependent function
\[ \Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{-i\left(kx - \frac{\hbar^2 k^2}{2m} t\right)} dx \]
\[ \Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{2\alpha}{\sqrt{2\pi k^2 + \alpha^2}} e^{-i\left(kx - \frac{\hbar^2 k^2}{2m} t\right)} dx \]
Evaluated Numerically!!!

14. Delta Function. Consider delta function as in the figure
\[ \delta(x) = \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases} \]
with the properties:
\[ \int_{-\infty}^{\infty} \delta(x) dx = 1; f(x) \delta(x - a) = f(a) \delta(x - a) \text{ and } \int_{-\infty}^{\infty} f(x) \delta(x - a) dx = f(a) \]
Obtain solution of the Schrödinger equation for the potential
\[ V(x) = -\alpha \delta(x) \]
Solution. It yields bound state for \( E < 0 \) and scattering state for \( E > 0 \). Let us obtain bound state solution: with this potential Schrödinger equation takes the form:
General solution of the equation:
\[- \frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - \alpha \delta(x) \psi = E \psi\]

where \( \kappa = \sqrt{\frac{2mE}{\hbar}} \) and it is positive. Then when \( x \to \pm \infty \) we obtain wave functions for \( x > 0 \) and \( x < 0 \):
\[\psi_+ = Ae^{-\kappa x} \quad \text{for} \quad x > 0 \]
\[\psi_- = Be^{\kappa x} \quad \text{for} \quad x < 0 \]

we can stitch the function together by using boundary condition at \( x = 0 \).

This condition leads to \( A = B \). Derivative of the functions should also be continuous at the boundary but, for infinite potential this continuity can be applied such that, \( \epsilon \to 0 \):
\[
\int_{-\epsilon}^{\epsilon} \frac{d^2\psi}{dx^2} \, dx = \left[ \frac{d\psi}{dx} \right]_{-\epsilon}^{\epsilon} = \Delta \left( \frac{d\psi}{dx} \right) = - \left( \frac{2m\alpha}{\hbar^2} \right) \psi(0)
\]
on the other hand:
\[\frac{d\psi_+}{dx} = -\alpha \kappa; x \to 0^+ \]
\[\frac{d\psi_-}{dx} = \alpha \kappa; x \to 0^- \]

Then \( \Delta \left( \frac{d\psi}{dx} \right) = -2\alpha \kappa = -\left( \frac{2m\alpha}{\hbar^2} \right) \psi(0) \). It is obvious that \( \psi(0) = A \) and \( \kappa = \frac{ma}{\hbar^2} \).

Then the allowed energy is \( E = -\frac{ma^2}{2\hbar^2} \). Finally normalization yields:
\[
\int_{-\infty}^{\infty} A^2 e^{-2\kappa x} \, dx = 2 \int_{0}^{\infty} A^2 e^{-2\kappa x} \, dx = 1 \Rightarrow A = \sqrt{\kappa} = \sqrt{\frac{ma}{\hbar^2}}
\]

Scattering state: \( E > 0 \). In this case the solution is given by:
\[\psi = Ae^{-ikx} + Be^{ikx}; \quad x < 0 \]
\[\psi = Fe^{-ikx} + Ge^{ikx}; \quad x > 0 \]

where \( k = \sqrt{\frac{2mE}{\hbar}} \) is positive. The continuity at \( x = 0 \) gives that:
\[A + B = F + G \]

derivative gives that
\[
\Delta \left( \frac{d\psi}{dx} \right) = ik(F - G - A + B) = - \left( \frac{2ma}{\hbar^2} \right) (A + B)
\]

Assume that the particle incident from left then the particle coming from left will be zero: \( G = 0 \). \( A \) is the amplitude of incident wave \( B \) is the amplitude of reflected wave and \( F \) is the amplitude of the transmitted wave. One can write:
\[B = \frac{i\beta}{1 - i\beta} A \quad \text{and} \quad F = \frac{1}{1 - i\beta} A; \quad \text{where} \quad \beta = \frac{ma}{\hbar^2 k} \]

Then the reflection and transmission coefficients are given by
\[R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1 + \beta^2}; \quad T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \beta^2}; \quad \text{with} \quad R + T = 1.\]
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1. Consider particles incident on a one-dimensional step function potential
   \[ V(x) = \begin{cases} 0 & \text{if } x < 0 \\ V_0 & \text{if } x > 0 \end{cases} \]
   with energy \( E > V \). Calculate the reflection and transmission coefficients for either direction of incidence. Consider the limits \( E \to V_0 \) and \( E \to \infty \).

**Solution 18. Incidence from the left.** In this case, solution of the Schrödinger equation yields the wave function:

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

Where

\[ k = \sqrt{\frac{2mE}{\hbar}}, \quad k' = \sqrt{\frac{2m}{\hbar} (E - V_0)} \]

Continuity of the wave function at \( x = 0 \) give:

\[ 1 + B = C ; \quad k(1 - B) = k'C \]

Solution of the equations for \( B \) and \( C \):

\[ B = \frac{k - k'}{k + k'}; \quad C = \frac{2k}{k + k'} \]

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

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

Reflection and transmission coefficients

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

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

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

\[ J_t + J_r = J_t \]

We check that

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

Incident from the right:

\[ \psi = \begin{cases} De^{-ikx} & x < 0 \\ e^{ikx} + Fe^{-ikx} & x > 0 \end{cases} \]

Continuity equations leads to the following expression for the reflection coefficients:

\[ R = |F|^2 = \left(\frac{k' - k}{k + k'}\right)^2 \]

Thus, we see that the reflection coefficient is independent of the direction of incidence.

Substitute values of \( k \) and \( k' \) into the reflection coefficient:

\[ R = \left(\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}}\right)^2 = \left(\frac{1 - \sqrt{1 - V_0/E}}{1 + \sqrt{1 - V_0/E}}\right)^2 \]

When \( E \to V_0; R \to 1 \); barrier becomes impenetrable.

When \( E \to \infty; R \to 0 \); barrier becomes irrelevant.

2. Solve the previous problem for \( E < V_0 \).

3. Consider a step function potential

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

and particles of energy \( E > V \) incident on it from both sides simultaneously. Its wave function is given by:

\[ \psi = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{ikx} + De^{-ikx} & x > 0 \end{cases} \]

(a) Determine two relations among the coefficients \( A, B, C \) and \( D \) from the continuity of the wave function and of its derivative at the point \( x = 0 \).

(b) Determine current densities.

(c) Write down conservation of current

\[ J^+ + J^\pm = J^- + J^\mp \]

in terms of \( A, D, k \) and \( k' \).

4. Consider a standard one-dimensional square potential barrier,

\[ V(x) = \begin{cases} 0 & \text{if } a < x < 0 \\ V_0 & \text{if } 0 < x < a \end{cases} \]
(a) Particles of energy \( E < V_0 \) are incident on it from the left. Calculate the transmission coefficient \( T \).
(b) How does \( T \) behave for very large energies? What is its low-energy limit?
(c) Are there any specific values of positive energy for which there is absolutely no reflection and the well is transparent? Verify explicitly that for these particular values the amplitude of the reflected wave vanishes.
(d) Is the transmission classically possible?

5. Consider a standard one-dimensional square potential well,

\[
V(x) = \begin{cases} 
0 & \text{if } -a/2 < x < a/2 \\
V_0 & \text{otherwise}
\end{cases}
\]

(a) Determine an equation for the eigenvalues of a particle in the well.
(b) Is energy continuous or discrete?
(c) The solution yields that: 
\[
\sqrt{\frac{V_0 - \epsilon}{\epsilon}} = \tan[\sqrt{2} \sqrt{\epsilon}]
\]
for the values \( a = 1, \hbar = 1, m = 1 \). For large values of \( V_0 \) determine energy of the particle. Compare your result energy of the particle given in the graph for large \( V_0 = 300 \) and energy of the particle in the infinite well potential.

\[
\left\{ \tan\left(\sqrt{\frac{2}{\epsilon}}\right), \sqrt{\frac{300 - \epsilon}{\epsilon}} \right\}
\]
6. If the particle is confined to a sphere of radius $a$, clearly the radial wavefunction which if finite at $r = 0$ is given by $j_l(kr)$ because $n_l(kr)$, unstable at the origin. The condition that it vanishes at $r = a$ requires that

$$j_l(ka) = 0$$

Thus the allowed energies are related to the zero's of the spherical Bessel functions. These are can be obtained from the following graphs. The numbers on the top of the graph represents values of $l$. Determine configuration of 20 spinless particle in the spherical well.