Tutorial 8 - Particle on a Ring, Scattering from Potential Barrier

Question 1:

Consider a particle of mass m that is moving on a one dimension on a ring of circumference L. The state of the particle is given by

$$\Psi(x,t) = \frac{1}{\sqrt{3L}} e^{i\left(\frac{2\pi}{L}x - \omega_0 t\right)} + \frac{1}{\sqrt{6L}} e^{i\left(\frac{4\pi}{L}x - 4\omega_0 t\right)} + \frac{A}{\sqrt{L}} e^{i\left(-\frac{2\pi}{L}x - \omega_0 t\right)}.$$

1. Find ω_0.
2. Find $|A|$.
3. What are the possible values of momentum which can be measured in the system and with what probability?
4. What are the possible values of energy which can be measured in the system and with what probability?
5. Calculate the expectation values for the momentum and the energy of the particle.

   In a measurement of the particle's energy we measured $E = \frac{2\hbar^2\pi^2}{mL^2}$.
6. What would be the state of the particle?
7. What are the possible values of momentum which can be measured in the system and with what probability?

Solution:

Recalling from the homework exercise:
The solution of the Schrödinger equation of a free particle,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \rightarrow \quad \frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where } k = \frac{\sqrt{2mE}}{\hbar}$$

is that of a combination of plane waves

$$\psi(x) \propto e^{\pm ikx}.$$

Applying the boundary condition, we find that

$$\psi(x) = \psi(x+L) \quad \rightarrow \quad e^{ikL} = 1 \quad \rightarrow \quad k \equiv k_n = \frac{2\pi n}{L}.$$

meaning that the stationary states of the system are a discrete set of plane waves

$$\psi_n(x) = N_n e^{ik_n x}, \quad \text{with } k_n = \frac{2\pi n}{L},$$

and the energy associated with each state is

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

The normalization condition yields

$$\langle\psi_m, \psi_n\rangle = \int_0^L N_m^* N_n e^{i\frac{2\pi}{L}x(n-m)} dx = N_m^* N_n L\delta_{nm} = \delta_{nm} \quad \text{if} \quad |N_n| = \frac{1}{\sqrt{L}}$$

Thus, the complete solution is of the form

$$\Psi(x,t) = \sum c_n \frac{1}{\sqrt{L}} e^{i\frac{2\pi n}{L}x} e^{-iE_n t/\hbar}$$

1. Using the solution for a free particle on a ring, we immediately see that (from the first term for example)

$$\boxed{\omega_0 = \frac{E_1}{\hbar} = \frac{2\pi^2\hbar}{mL^2}}.$$

2. Using the normalization condition for the wave function

$$\Psi(x,t) = \frac{1}{\sqrt{3}}\psi_1 e^{-iE_1 t/\hbar} + \frac{1}{\sqrt{6}}\psi_2 e^{-iE_2 t/\hbar} + A\psi_{-1} e^{-iE_1 t/\hbar}$$

$$\langle\Psi|\Psi\rangle = \frac{1}{3} + \frac{1}{6} + |A|^2 = 1 \quad \to \quad \boxed{|A| = \frac{1}{\sqrt{2}}}.$$

3. Since ψ_n are the eigenfunctions of the Hamiltonian $\hat{H} = \hat{p}^2/2m$, which in the case of a free particle are also the eigenfunctions of definite momentum $\left(\langle p^2\rangle = \langle p\rangle^2\right)$, thus

$$\langle p\rangle_n = \sqrt{2mE_n} = \hbar k_n = \frac{2\pi\hbar n}{L}.$$

In our case the only eigenfunctions with nonzero probability are $n = \pm 1, 2$, for which the probabilities are

$$P\left(\langle p\rangle = \frac{2\pi\hbar}{L}\right) = \frac{1}{3},$$
$$P\left(\langle p\rangle = -\frac{2\pi\hbar}{L}\right) = \frac{1}{2},$$
$$P\left(\langle p\rangle = \frac{4\pi\hbar}{L}\right) = \frac{1}{6}.$$

4. We've seen that the Hamiltonian's eigenvalues are $E_n = \frac{2\pi^2\hbar^2 n^2}{mL^2}$, and they are degenerate for $\pm n$. Thus

$$P\left(E = \frac{2\pi^2\hbar^2}{mL^2}\right) = P(n=1) + P(n=-1) = \frac{5}{6},$$
$$P\left(E = \frac{8\pi^2\hbar^2}{mL^2}\right) = P(n=2) = \frac{1}{6}.$$

5. The expectation value of an observable $\hat{Q}$ is

$$\langle Q\rangle = \sum_n q_n |c_n|^2,$$

for the energy and momentum it reads

$$\langle E\rangle = \frac{2\pi^2\hbar^2}{mL^2}\left(\frac{5}{6} + 4\frac{1}{6}\right) = \frac{3\pi^2\hbar^2}{mL^2},$$
$$\langle p\rangle = \frac{2\pi\hbar}{L}\left(\frac{1}{3} - \frac{1}{2} + 2\frac{1}{6}\right) = \frac{\pi\hbar}{3L}.$$

6. Measuring $E = \frac{2\pi^2\hbar^2}{mL^2}$ corresponds to $\psi_{\pm 1}$, hence the wave function right after the measurement is

$$\Psi'(x,t) = A\left(c_1\psi_1 + c_{-1}\psi_{-1}\right)e^{-iEt/\hbar},$$

where $c_{\pm 1}$ are determined from the initial wave function and normalization condition

$$\Psi(x,0) = \frac{1}{\sqrt{3}}\psi_1 + \frac{1}{\sqrt{6}}\psi_2 + \frac{1}{\sqrt{2}}\psi_{-1} \quad \to \quad \begin{cases} c_1 = \langle\psi_1|\Psi(x,0)\rangle = \frac{1}{\sqrt{3}}, \\ c_{-1} = \langle\psi_{-1}|\Psi(x,0)\rangle = \frac{1}{\sqrt{2}}, \end{cases}$$

and

$$|A|^2\left(\frac{1}{3}+\frac{1}{2}\right)=1 \quad\rightarrow\quad |A|=\sqrt{\frac{6}{5}}.$$

Thus, the state of the particle is

$$\boxed{\Psi'(x,t)=\left(\sqrt{\frac{2}{5}}\psi_1+\sqrt{\frac{3}{5}}\psi_{-1}\right)e^{-iEt/\hbar}}.$$

7. Similar to (3), we have

$$P\left(\langle p\rangle=\frac{2\pi\hbar}{L}\right)=\frac{2}{5},$$
$$P\left(\langle p\rangle=-\frac{2\pi\hbar}{L}\right)=\frac{3}{5}.$$

Question 2:

Consider a particle on a one dimensional ring of circumference L, with the periodic boundary conditions $\psi(x+L)=\psi(x)$. In addition, there is a potential well of the form $V(x)=-g\delta(x-L/2)$, where g is a positive constant.

1. Find the bound states solution ($E<0$).
2. Write the boundary conditions and attain an equation for the energy of the particle.
3. Are there bound states for all values of g and L? Explain.

Solution:

Let us use a symmetric coordinate system where ψ is periodic between $[-L/2,L/2]$ and the potential is $V(x)=-g\delta(x)$.

1. The time-independent Schrödinger equation, for $E<0$, everywhere except for $x=0$ reads

$$\frac{d^2\psi}{dx^2}=\kappa^2\psi,\qquad \text{where}\qquad \kappa=\frac{\sqrt{2m|E|}}{\hbar}\qquad \text{is real.}$$

The solutions are

$$\psi(x)=\begin{cases}Ae^{-\kappa x}+Be^{\kappa x}, & -\frac{L}{2}<x<0,\\ Ce^{-\kappa x}+De^{\kappa x}, & 0<x<\frac{L}{2}.\end{cases}$$

Applying the periodic boundary conditions and the continuity of $\psi(x)$ at $x=0$ yield

$$\psi\left(-\frac{L}{2}\right)=\psi\left(\frac{L}{2}\right)\quad\rightarrow\quad Ae^{\kappa L/2}+Be^{-\kappa L/2}=Ce^{-\kappa L/2}+De^{\kappa L/2}\quad\rightarrow\quad A-D=e^{\kappa L}(C-B),$$
$$\psi(0_-)=\psi(0_+)\quad\rightarrow\quad A+B=C+D\quad\rightarrow\quad A-D=C-B,$$

which imply that $A=D$ and $B=C$,

$$\psi(x)=\begin{cases}Ae^{-\kappa x}+Be^{\kappa x}, & -\frac{L}{2}<x<0,\\ Be^{-\kappa x}+Ae^{\kappa x}, & 0<x<\frac{L}{2}.\end{cases}$$

In addition we have the boundary condition for the derivative of ψ,

$$\psi'\left(-\frac{L}{2}\right)=\psi'\left(\frac{L}{2}\right)\quad\rightarrow\quad -Ae^{\kappa L/2}+Be^{-\kappa L/2}=Ae^{\kappa L/2}-Be^{-\kappa L/2}\quad\rightarrow\quad B=Ae^{\kappa L},$$

which gives us the bound state solution

$$\boxed{\psi(x)=\begin{cases}A\left(e^{-\kappa x}+e^{\kappa(x+L)}\right), & -\frac{L}{2}<x<0,\\ A\left(e^{-\kappa(x-L)}+e^{\kappa x}\right), & 0<x<\frac{L}{2}.\end{cases}}$$

2. Next we use the integrated Schrödinger equation around $x = 0$, which reads

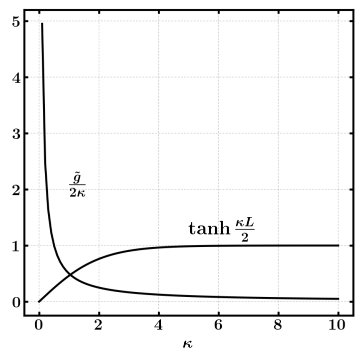
$$\int_{-\epsilon}^{\epsilon} \frac{d^2\psi}{dx^2} dx = -\frac{2m}{\hbar^2} \int_{-\epsilon}^{\epsilon} g\delta(x)\psi dx + \int_{-\epsilon}^{\epsilon} \kappa^2 \psi dx \quad \rightarrow \quad \psi'(0_+) - \psi'(0_-) = -\tilde{g}\psi(0),$$

where $\tilde{g} \equiv \frac{2mg}{\hbar^2}$ which, when plugging in the wave function, yields

$$\kappa\left[1 - e^{\kappa L} - \left(e^{\kappa L} - 1\right)\right] = -\tilde{g}\left(1 + e^{\kappa L}\right) \quad \rightarrow \quad \boxed{\frac{\tilde{g}}{2\kappa} = \frac{e^{\kappa L/2} - e^{-\kappa L/2}}{e^{\kappa L/2} + e^{-\kappa L/2}} = \tanh\frac{\kappa L}{2}},$$

which, recalling that κ depends on E, is the transcendental equation for the allowed energies.

3. Plotting the functions of κ in both sides of the equation above looks like



where we set $\tilde{g} = 1$ and $L = 1$. It is clear that there is always a single value of allowed energy for all g and L, since there will always be a crossing point.

Question 3:

Consider a potential barrier given by $V(x) = V_0\Theta(x)$ and particles with $E > V_0$ incident on it. Find reflection coefficient for particles incident from the right and for particles incident from the right. Discuss the limits $E \rightarrow V_0$ and $E \rightarrow \infty$.

Solution:

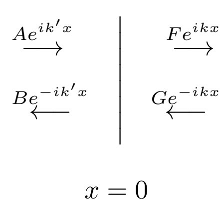
The Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi \quad \rightarrow \quad \begin{cases} \frac{d^2\psi}{dx^2} = -k'^2\psi, & x < 0, \text{ where } k' \equiv \frac{\sqrt{2mE}}{\hbar} \quad \text{is real,} \\ \frac{d^2\psi}{dx^2} = -k^2\psi, & x > 0, \text{ where } k \equiv \frac{\sqrt{2m(E-V_0)}}{\hbar} \quad \text{is real.} \end{cases}$$

The solution to this equation is of the form

$$\psi(x) = \begin{cases} Ae^{ik'x} + Be^{-ik'x}, & x < 0, \\ Fe^{ikx} + Ge^{-ikx}, & x > 0, \end{cases}$$

Since we consider a particle that propagates from the right (i.e. from $x \rightarrow \infty$ towards $x = 0$), which amplitude is represented by G, we have no reflection in the region $x < 0$, hence $A = 0$.



Using the boundary conditions at $x = 0$ we have

$$\psi(0_-) = \psi(0_+): \quad B = F + G,$$
$$\psi'(0_-) = \psi'(0_+): \quad -k'B = k(F - G),$$

$$(k-k')\,G=(k+k')\,F$$

which gives us

$$F=\frac{k-k'}{k'+k}G \quad \text{and} \quad B=\frac{2k}{k'+k}G.$$

The reflection and transmission coefficients are determined from the probability density currents:

$$R=\frac{|J_r|}{|J_i|} \quad \text{and} \quad T=\frac{|J_t|}{|J_i|}.$$

It is easy to calculate the currents

$$\begin{aligned}
J_i &= \frac{\hbar}{m}\mathrm{Im}\left[\psi_i^*\frac{\partial\psi_i}{\partial x}\right] = -\frac{\hbar k}{m}\,|G|^2\,, \\
J_r &= \frac{\hbar}{m}\mathrm{Im}\left[\psi_r^*\frac{\partial\psi_r}{\partial x}\right] = \frac{\hbar k}{m}\,|F|^2 = \frac{\hbar k}{m}\left|\frac{k-k'}{k'+k}G\right|^2, \\
J_t &= \frac{\hbar}{m}\mathrm{Im}\left[\psi_t^*\frac{\partial\psi_t}{\partial x}\right] = -\frac{\hbar k'}{m}\,|B|^2 = -\frac{\hbar k'}{m}\left|\frac{2k}{k'+k}G\right|^2,
\end{aligned}$$

thus

$$\boxed{R=\left|\frac{k'-k}{k'+k}\right|^2=\frac{(k'-k)^2}{(k'+k)^2} \quad \text{and} \quad T=\frac{k'}{k}\left|\frac{2k}{k'+k}\right|^2=\frac{4kk'}{(k'+k)^2}}.$$

In the limits, we find

$$\begin{aligned}
E\to V_0: &\quad R\to 1 \quad \text{and} \quad T\to 0, \\
E\to\infty: &\quad R\to 0 \quad \text{and} \quad T\to 1,
\end{aligned}$$

as one would anticipate, at high energies the potential is transparent, however at $E=V_0$ somehow we get a complete reflection.
In this case ($E>V_0$), the solution is the same for a particle from the left as it is for a particle from the right.

Question 4:

Consider a potential barrier given by $V(x)=V_0\Theta(x)$ and particles with $0<E<V_0$ incident on it from the left. Find the reflection coefficient.

Solution:

The Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V_0\psi=E\psi \quad \to \quad \begin{cases} \frac{d^2\psi}{dx^2}=-k^2\psi, & x<0,\text{ where } k\equiv\frac{\sqrt{2mE}}{\hbar} \text{ is real,} \\ \frac{d^2\psi}{dx^2}=\kappa^2\psi, & x>0,\text{ where } \kappa\equiv\frac{\sqrt{2m(V_0-E)}}{\hbar} \text{ is real.}\end{cases}$$

The solution to this equation is of the form

$$\psi(x)=\begin{cases} Ae^{ikx}+Be^{-ikx}, & x<0, \\ Fe^{\kappa x}+Ge^{-\kappa x}, & x>0.\end{cases}$$

Since a diverging wave function at $x\to\infty$ is non physical we require $F=0$. Using the boundary conditions at $x=0$ we have

$$\begin{aligned}
\psi(0_-)=\psi(0_+): &\quad A+B=G, \\
\psi'(0_-)=\psi'(0_+): &\quad ik(A-B)=-\kappa G,
\end{aligned}$$

which gives us

$$B=-\frac{\kappa+ik}{\kappa-ik}A \quad \text{and} \quad G=-\frac{2ik}{\kappa-ik}A.$$

The reflection and transmission coefficients are

$$R = \frac{|B|^2}{|A|^2} = 1 \quad \text{and} \quad T = 0,$$

which is similar to the classical case, however, there is a nonzero probability for "finding" the particle inside the barrier. Thus, when we will consider a spatially finite barrier we can expect to find a nonzero transmission coefficient.