PHSX 711: Homework #4

October 3, 2024

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Problem 1

(5 pts) (Shankar) Exercise 5.2.2 part (a) only
Exercise 5.2.2* (a) Show that for any normalized $|\psi\rangle$, $\langle\psi|H|\psi\rangle \geq E_0$, where E_0 is the lowest-energy eigenvalue. (Hint: Expand $|\psi\rangle$ in the eigenbasis of H.)

Solution:

$$\begin{aligned}
\langle\psi|H|\psi\rangle &= \int_{-\infty}^{\infty} \langle\psi|H|n\rangle \langle n|\psi\rangle \; dn \\
&= \int_{-\infty}^{\infty} E_n \langle\psi|n\rangle \langle n|\psi\rangle \; dn \\
&\geq \int_{-\infty}^{\infty} E_0 \langle\psi|n\rangle \langle n|\psi\rangle \; dn \\
&\geq E_0 \langle\psi|\psi\rangle \\
&\geq E_0
\end{aligned}$$

Problem 2

(15 pts) Exercise 5.2.6 (Shankar)
Exercise 5.2.6* Square Well Potential. Consider a particle in a square well potential:

$$V(x) = \begin{cases} 0, & |x| \leq a \\ V_0, & |x| > a \end{cases}$$

Since when $V_0 \to \infty$, we have a box, let us guess what the lowering of the walls does to the states. First of all, all the bound states (which alone we are interested in), will have $E \leq V_0$. Second, the wave functions of the low-lying levels will look like those of the particle in a box, with the obvious difference that ψ will not vanish at the walls but instead spill out with an exponential tail. The eigenfunctions will still be even, odd, even, etc.

(1) Show that the even solutions have energies that satisfy the transcendental equation

$$k \tan ka = \kappa \tag{5.2.23}$$

while the odd ones will have energies that satisfy

$$k \cot ka = -\kappa \tag{5.2.24}$$

where k and κ are the real and complex wave numbers inside and outside the well, respectively. Note that k and κ are related by

$$k^2 + \kappa^2 = 2mV_0/\hbar^2 \tag{5.2.25}$$

Solution (I swap k and κ):

We have the wavefunction

$$\frac{\hbar}{2m}\psi'' + V(x)\psi = (E)\psi$$

$$\begin{cases} \psi''(x) &= -k^2\psi, \quad k \equiv \frac{\sqrt{2mE}}{\hbar}, \quad \text{for } |x| < a \\ \psi''(x) &= \kappa^2\psi, \quad \kappa \equiv \frac{\sqrt{2m(V_0-E)}}{\hbar}, \quad \text{for } |x| > a \end{cases}$$

This gives exponential solutions in Regions I and III where there is a potential, and sin/cos solutions in region II.

$$\begin{aligned} |\psi_I(x)\rangle &= Ae^{-kx} + Be^{kx} \\ |\psi_{II}(x)\rangle &= Ce^{-i\kappa x} + De^{i\kappa x} \\ |\psi_{III}(x\rangle &= Fe^{-kx} + Ge^{kx} \end{aligned}$$

The condition of finiteness demands that $B = G = 0$. The condition of continuity demands that $|\psi_I(-a)\rangle = |\psi_{II}(-a)\rangle$ and $|\psi_{II}(a)\rangle = |\psi_{III}(x(a)\rangle$. This potential is an even function, so we can assume that the solutions are either even or odd.

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i. **Even solutions:**

$$|\psi\rangle = \begin{cases} Ae^{-kx}, & \text{(x>a)} \\ D\cos(\kappa x), & \text{(0<x<a)} \\ \psi(-x), & \text{(x<0)} \end{cases}$$

Continuity tells us that

$$Fe^{-ka} = D\cos(\kappa a)$$
$$-Fe^{-ka} = -D\sin(\kappa a)$$

Dividing the two gives us a relation which allows us to solve for energies:

$$k = \kappa\tan(\kappa a)$$

ii. **Odd solutions:**

$$|\psi\rangle = \begin{cases} Ae^{-kx}, & \text{(x>a)} \\ D\sin(\kappa x), & \text{(0<x<a)} \\ \psi(-x), & \text{(x<0)} \end{cases}$$

Continuity tells us that

$$Fe^{-ka} = C\sin(\kappa a)$$
$$-Fe^{-ka} = C\cos(\kappa a)$$

Dividing the two gives us a relation which allows us to solve for energies:

$$-k = \kappa\cot(\kappa a)$$

(2) Equations (5.2.23) and (5.2.24) must be solved graphically. In the $(a = ka, \beta)$ plane, imagine a circle that obeys Eq. (5.2.25). The bound states are then given by the intersection of the curve $\alpha\tan\alpha = \beta$ or $\alpha\cot\alpha = -\beta$ with the circle. (Remember α and β are positive.)

Solution:

$$k = \kappa\tan(\kappa a), \qquad \text{(even)}$$
$$-k = \kappa\cot(\kappa a), \qquad \text{(odd)}$$

let

$$\begin{cases} z & = & \kappa a \\ z' & = & ka \\ z_0 & = & \frac{a}{\hbar}\sqrt{2mV_0} \\ z^2 + z_0^2 & = & \frac{2ma^2V_0}{\hbar^2} \end{cases}$$

Valid energies are given by

$$\begin{cases} z' & = & z\tan z \\ z' & = & -z\cot z \end{cases}$$

Problem 2 continued on next page...

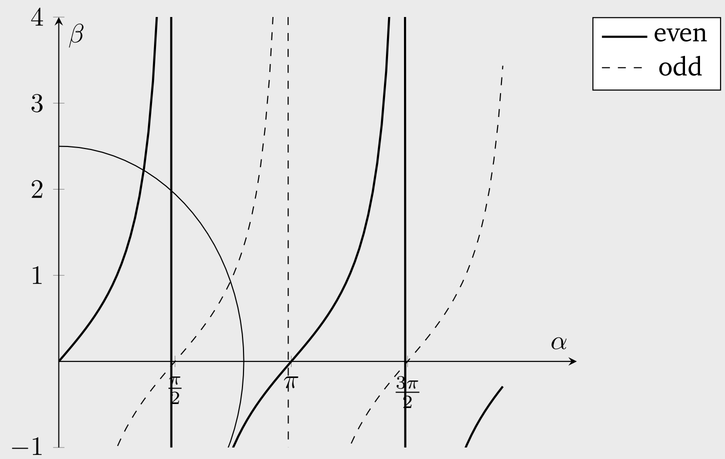

Figure 1: Plot for odd and even solutions of $\beta = \alpha \tan(\alpha)$ and $\beta = -\alpha \cot(\alpha)$

(3) Show that there is always one even solution and that there is no odd solution unless $V_0 > \hbar^2\pi^2/8ma^2$. What is E when V_0 just meets this requirement? Note that the general result from Exercise 5.2.2b holds.

Solution:

Graphically there is always going to be at least 1 intersection between our circle and the odd solution curve, however if the radius of the circle is small enough there may not be a solution for the odd solutions. It happens that when $V_0 > \frac{\hbar^2\pi^2}{8ma^2}$ there exist only even solutions.

Hint: For part (2), make a simple sketch to show the 3 curves (5.2.23-5.2.25). Then, you should be able to solve (3) rather easily by inspecting the figure you draw. (no complicated calculation or precise plotting is needed).

Problem 3

(5 pts) 3. Exercise 5.3.4 (Shankar)
Exercise 5.3.4* Consider $\psi = Ae^{i\alpha x/\hbar} + Be^{-i\alpha x/\hbar}$ in one dimension. Show that $j = (|A|^2 - |B|^2)\alpha/m$. The absence of cross terms between the right- and left-moving pieces in ψ allows us to associate the two parts of j with corresponding parts of ψ.

Solution:
j refers to the current density of this wave function. In electromagnetism we have the continuity equation which states that any decrease of charge in a volume equals the flow of charge out of it.

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \vec{j}$$

$$\frac{\partial \rho}{\partial t} = i\hbar \frac{\partial \psi^* \psi}{\partial t} = -\nabla \cdot \vec{j}$$

$$\frac{\partial \rho}{\partial t} = -\frac{\hbar}{2mi} \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*)$$

So therefore:

$$\vec{j} = \frac{\hbar}{2mi} (\psi^* \nabla \psi - \psi \nabla \psi^*)$$

$$\begin{cases} \nabla \psi & = & A\frac{i\alpha}{\hbar}e^{i\alpha x/\hbar} - B\frac{i\alpha}{\hbar}e^{-i\alpha x/\hbar} \\ \nabla \psi^* & = & -A\frac{i\alpha}{\hbar}e^{-i\alpha x/\hbar} + B\frac{i\alpha}{\hbar}e^{i\alpha x/\hbar} \end{cases}$$

$$\begin{aligned} \psi^* \nabla \psi &= \left(Ae^{-i\alpha x/\hbar} + Be^{i\alpha x/\hbar}\right)\left(A\frac{i\alpha}{\hbar}e^{i\alpha x/\hbar} - B\frac{i\alpha}{\hbar}e^{-i\alpha x/\hbar}\right) \\ &= A^2\frac{i\alpha}{\hbar} - B^2\frac{i\alpha}{\hbar} \\ &= \frac{i\alpha}{\hbar}\left(A^2 - B^2\right) \end{aligned}$$

$$\begin{aligned} \psi \nabla \psi^* &= \left(Ae^{i\alpha x/\hbar} + Be^{-i\alpha x/\hbar}\right)\left(-A\frac{i\alpha}{\hbar}e^{-i\alpha x/\hbar} + B\frac{i\alpha}{\hbar}e^{i\alpha x/\hbar}\right) \\ &= -A^2\frac{i\alpha}{\hbar} + B^2\frac{i\alpha}{\hbar} \\ &= \frac{i\alpha}{\hbar}(B^2 - A^2) \end{aligned}$$

$$\begin{aligned} \vec{j} &= \frac{\hbar}{2mi}\left(\frac{i\alpha}{\hbar}\right)\left([A^2 - B^2] - [-A^2 + B^2]\right) \\ &= \frac{\cancel{\hbar}}{2m\cancel{i}}\left(\frac{\cancel{i}\alpha}{\cancel{\hbar}}\right)\left([A^2 - B^2] + [A^2 - B^2]\right) \\ &= \frac{\alpha}{2m}\left(2[A^2 - B^2]\right) \\ &= \frac{\alpha}{m}[|A|^2 - |B|^2] \end{aligned}$$