5401 Problem Set 4

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Question I.

Shankar Exercise 5.2.6

Square Well Potential. Consider a particle in a square well potential:

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

Since when $V_0 \to \infty$, we have a box, let us guess what the lowering of the walls does to the states. Fist 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

$$k \tan ka = \kappa$$

while the odd ones will have energies that satisfy

$$k \cot ka = -\kappa$$

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

$$k^2 + \kappa^2 = 2mV_0/\hbar^2$$

Verify that as V_0 tends to ∞, we regain the levels in the box.

Solving for the energy eigenstates of $\hbar\psi'' = 2m(E - V(x))\psi$ for $E \leq V_0$ in each region give:

$$\begin{aligned}
\psi_I &= Ae^{-\kappa x} + Be^{\kappa x} \quad x < -a \\
\psi_{II} &= Ce^{ikx} + De^{-ikx} \quad |x| < a \\
\psi_{III} &= Ee^{-\kappa x} + Fe^{\kappa x} \quad x > a \\
\kappa &= \frac{\sqrt{2m(V_0 - E)}}{\hbar} \\
k &= \frac{\sqrt{2mE}}{\hbar}
\end{aligned}$$

Immediately it is required for a normalizable state that $A = F = 0$. We also have that ψ and its first derivative are to be continuous on the boundaries $|x| = a$, so we have:

$$\begin{aligned} Be^{-\kappa a} &= Ce^{-ika} + De^{ika} \\ \kappa Be^{-\kappa a} &= ikCe^{ika} - ikDe^{ika} \\ Ee^{-\kappa a} &= Ce^{ika} + De^{-ika} \\ -\kappa Ee^{-\kappa a} &= ikCe^{ika} - ikDe^{-ika} \end{aligned}$$

Looking now at the even solutions, we have $B = E$ and $C = D$, so:

$$\begin{aligned} Be^{-\kappa a} &= Ce^{-ika} + Ce^{ika} \\ \kappa Be^{-\kappa a} &= ikCe^{ika} - ikCe^{ika} \end{aligned}$$

or

$$\begin{bmatrix} e^{-\kappa a} & -2\cos ka \\ \kappa e^{-\kappa a} & -2k\sin ka \end{bmatrix} \begin{bmatrix} B \\ C \end{bmatrix} = 0$$

This system is solvable if the determinant of the coefficient matrix vanishes, implying the given result

$$k \tan ka = \kappa$$

The odd solutions follow similarly with the conditions that $B = -E$ and $C = -D$, and we get the system:

$$\begin{bmatrix} e^{-\kappa a} & -2i\sin ka \\ \kappa e^{-\kappa a} & -2ik\cos ka \end{bmatrix} \begin{bmatrix} B \\ C \end{bmatrix} = 0$$

This again yields the given result:

$$k \cot ka = -\kappa$$

2. Equations (5.2.23) and (5.2.23) must be solved graphically. In the ($\alpha = ka, \beta = \kappa a$) 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.)

   The plot for this is given in Figure 1, where the red curves are odd states and the green curves are even states

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

   For the case $V_0 \to 0$, the circle will always intersect at least the first even solution. For the case $V_0 = \hbar^2\pi^2/8ma^2$, this implies $E = \hbar^2k^2/2m$.

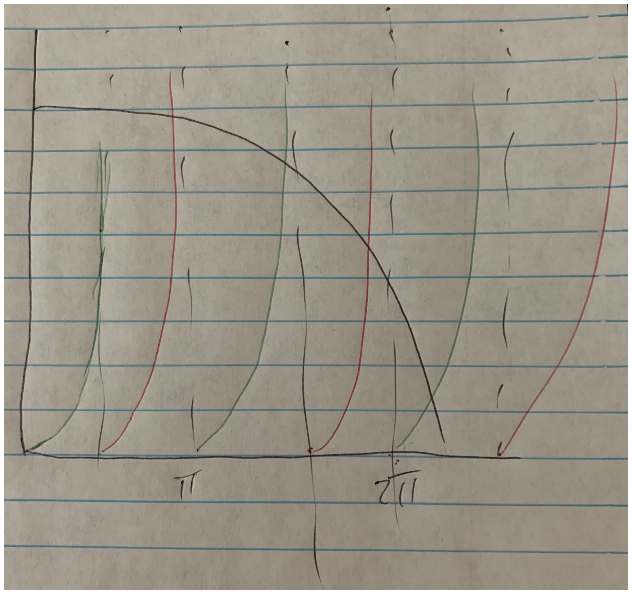

Figure 1: Figure for question I part 2

Question II.

Shankar Exercise 5.3.3

Consider

$$\psi_{\mathbf{p}} = \left(\frac{1}{2\pi\hbar}\right)^{3/2} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$$

Find $\mathbf{j}$ and P and compare the relation between them to the electromagnetic equation $\mathbf{j} = \rho\mathbf{v}$, $\mathbf{v}$ being the velocity. Since ρ and $\mathbf{j}$ are constant, note that the continuity Eq. (5.3.7) is trivially satisfied.

From the continuity equation we have:

$$\begin{aligned}
\boldsymbol{\nabla} e^{i(\mathbf{p}\cdot\mathbf{r}/\hbar)} &= \frac{i\mathbf{p}}{\hbar} e^{i(\mathbf{p}\cdot\mathbf{r}/\hbar)} \\
\mathbf{j} &= \frac{\hbar}{2mi}(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*) \\
&= \left(\frac{1}{2m\hbar}\right)^3 \frac{\mathbf{p}}{m} \\
p &= \psi^*\psi \\
&= \left(\frac{1}{2m\hbar}\right)^3 \\
\implies \mathbf{j} &= p\frac{\mathbf{p}}{m}
\end{aligned}$$

This is equivalent to the statement of $\mathbf{j} = \rho\mathbf{v}$, where $\mathbf{v} = \mathbf{p}/m$. This trivially satisfies continuity: $\frac{\mathrm{d}p}{\mathrm{d}t} = -\boldsymbol{\nabla}\mathbf{j}$.

Question III.

Shankar Exercise 5.3.4

Conside $\psi = Ae^{ipx/\hbar} + Be^{-ipx/\hbar}$ in one dimension. Show that $j = (|A|^2 + |B|^2)p/m$. 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.

If we take $\psi^* \frac{\partial}{\partial x}\psi - \psi\frac{\partial}{\partial x}\psi^*$ and simplify we get:

$$\begin{aligned} \psi^* \frac{\partial}{\partial x}\psi - \psi\frac{\partial}{\partial x}\psi^* &= \frac{2ip}{\hbar}(|A|^2 - |B|^2) \\ j &= \frac{\hbar}{2mi}(\psi^* \frac{\partial}{\partial x}\psi - \psi\frac{\partial}{\partial x}\psi^*) \\ &= \frac{p}{m}(|A|^2 - |B|^2) \end{aligned}$$

Question IV.

Shankar Exercise 5.4.2

(a) Calculate R and T for scattering off a potential $V(x) = V_0 a\delta(x)$.

We denote region I as the negative side of the potential and region II as the positive side. We know that the wavefunctions must vanish on the boundary and we know $\psi'_{II} - \psi'_I = \frac{2m}{\hbar}V_0 a\psi(0)$. For $x \neq 0$ we have:

$$\begin{aligned} \psi'' + k^2\psi &= 0 \\ k &= \sqrt{\frac{2m}{\hbar^2}E} \end{aligned}$$

So we get the solutions:

$$
\begin{aligned}
\psi_I &= e^{ikx} + re^{-ikx} \\
\psi_{II} &= te^{ikx} \\
1 + r &= t \\
ikt - ik + ikr &= \frac{2m}{\hbar^2} V_0 at \\
t &= \frac{1}{1 + \frac{imV_0 a}{k\hbar^2}} \\
r &= \frac{-\frac{imV_0 a}{k\hbar^2}}{1 + \frac{imV_0 a}{k\hbar^2}} \\
R &= |r|^2 \\
&= \frac{1}{1 + \frac{2\hbar^2 E}{ma^2 V_0^2}} \\
T &= 1 - R \\
&= \frac{1}{1 + \frac{ma^2 V_0^2}{a\hbar^2 E}}
\end{aligned}
$$

(b) Do the same for the case $V = 0$ for $|x| > a$ and $V = V_0$ for $|x| < a$. Assume that the energy is positive but less than V_0.

In this case, we have three regions. region I will be negative of the potential, II will be in the potential, and III will be positive of the potential. We now get in regions I and III:

$$
\begin{aligned}
\psi'' + k^2\psi = 0 \\
\psi_I &= e^{ikx} + re^{-ikx} \\
\psi_{III} &= te^{ikx}
\end{aligned}
$$

In region II:

$$
\begin{aligned}
\psi'' + \kappa^2\psi = 0 \\
\kappa &= \sqrt{\frac{2m}{\hbar^2}(V_0 - E)} \\
\psi_{II} &= Ae^{\kappa x} + Be^{-\kappa x}
\end{aligned}
$$

Applying boundary conditions:

$$
\begin{aligned}
e^{-ika} + re^{ika} &= Ae^{-\kappa a} + Be^{\kappa a} \\
ike^{-ika} - ikre^{ika} &= \kappa Ae^{-\kappa a} - \kappa Be^{\kappa a} \\
te^{ika} &= Ae^{\kappa a} + Be^{-\kappa a} \\
ikte^{ika} &= \kappa Ae^{\kappa a} - \kappa Be^{-\kappa a}
\end{aligned}
$$

This yields some rather ugly transmission and reflection coefficients:

$$\begin{aligned}
t &= \frac{4e^{-2ika}}{4\cosh 2ka + \left(\frac{\kappa}{ik} + \frac{ik}{\kappa}\right) 2\sinh 2ka} \\
T &= |t|^2 \\
&= \frac{1}{1 + \frac{1}{4}\sinh^2 2ka \left(\frac{k^2+\kappa^2}{k\kappa}\right)^2} \\
R &= 1 - T \\
&= \frac{\frac{1}{4}\sinh^2 2ka \left(\frac{k^2+\kappa^2}{k\kappa}\right)^2}{1 + \frac{1}{4}\sinh^2 2ka \left(\frac{k^2+\kappa^2}{k\kappa}\right)^2}
\end{aligned}$$

Question V.

January 2019 Quantum Mechanics Prelim Problem 2

Take two hermitian operators $\hat{x}$ and $\hat{p}$ such that $[\hat{x}, \hat{p}] = i\hbar$. The spectrum of $\hat{x}$ is continuous and we have $\hat{x}\,|x\rangle = x\,|x\rangle, \quad x \in \mathbb{R}$. Also, the orthonormal basis states are normalized according to $\langle x'|x\rangle = \delta(x' - x)$.

(a) Show that $[\hat{x}, \hat{p}^n] = i\hbar\hat{p}^{n-1}$ holds true for positive integers n, and that $\left[\hat{x}, e^{-\frac{i\lambda\hat{p}}{\hbar}}\right] = \lambda e^{-\frac{i\lambda\hat{p}}{\hbar}}$. Henceforth assume that $\lambda \in \mathbb{R}$.

We know for a general commutator $[A, B^n] = nB^{n-1}[A, B]$. We know $[\hat{x}, \hat{p}] = i\hbar$, so the given relation holds $[\hat{x}, \hat{p}^n] = i\hbar\hat{p}^{n-1}$. For the second commutator, we have the generalization $\left[A, e^{\lambda}B\right] = \lambda[A, B]e^{\lambda B}$. From this and the previous relation we immediately get the relation given: $\left[\hat{x}, e^{-\frac{i\lambda\hat{p}}{\hbar}}\right] = \lambda e^{-\frac{i\lambda\hat{p}}{\hbar}}$.

(b) Show that $e^{-\frac{i\lambda\hat{p}}{\hbar}}\,|x\rangle$ is an eigenvector of the operator $\hat{x}$ with the eigenvalue $x + \lambda$. In fact, it is possible to choose the phase factors of the basis states $|x\rangle$ so that $e^{-\frac{i\lambda\hat{p}}{\hbar}}\,|x\rangle = |x = \lambda\rangle$; assume this has been done.

Using the result from part a, we can say:

$$\begin{aligned}
\hat{x}e^{-\frac{i\lambda\hat{p}}{\hbar}} &= e^{-\frac{i\lambda\hat{p}}{\hbar}}\hat{x} + \left[\hat{x}, e^{-\frac{i\lambda\hat{p}}{\hbar}}\right] \\
&= e^{-\frac{i\lambda\hat{p}}{\hbar}}\hat{x} + \lambda e^{-\frac{i\lambda\hat{p}}{\hbar}}
\end{aligned}$$

Acting on the vector $|x\rangle$:

$$\left(e^{-\frac{i\lambda\hat{p}}{\hbar}}\hat{x} + \lambda e^{-\frac{i\lambda\hat{p}}{\hbar}}\right)|x\rangle = e^{-\frac{i\lambda\hat{p}}{\hbar}}(x + \lambda)\,|x\rangle$$

Since the exponential factor is simply a rotation, we see that this is an eigenvector of eigenvalue $x + \lambda$.

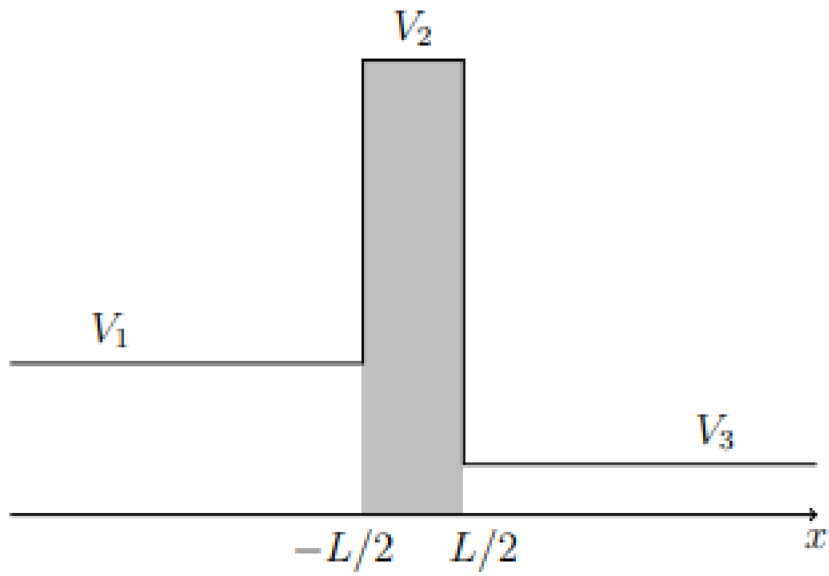

Figure 2: Potential for VI

(c) Show that $\langle x|\hat{p}|x'\rangle = \frac{\hbar}{i}\delta(x-x')$, proportional to the derivative of the delta function. Hint: express $\hat{p}$ as a derivative of $e^{-\frac{i\lambda\hat{p}}{\hbar}}$.

Noting that $\hat{p} = i\hbar\frac{\partial}{\partial x}$, we have $\langle x|\hat{p}|x'\rangle = \langle x|i\hbar\frac{\partial}{\partial x}|x'\rangle$. Noting that $\frac{\partial x'}{\partial x} = \delta(x-x')$, we take the conjugate and act on $\langle x|$ to get the given result $\langle x|\hat{p}|x'\rangle = \frac{\hbar}{i}\delta(x-x')$.

(d) What does the result in (c) say about momentum operator in position representation?

This result says that the momentum operator is antihermitian in the position representation.

Question VI.

January 2019 Quantum Mechanics Prelim Problem 3

A potential barrier V_2 of width L is centered around $x = 0$ between regions with constant potential V_1 for $x \leq -L/2$ and V_3 for $x \geq L/2$ with $V_3 > V_1$. The subscripts are used to consistently label the three regions with different potentials.

A particle of mass m is sent in from $x = -\infty$, traveling towards the right with energy E. The wave-function of the incoming particle is $\psi_{in} = Ae^{ik_1 x}$.

(a) What are the wave-functions in the three different regions for $E < V_2$?

This question carries out similarly to question IV with a different potential. We have three regions: regions I, II, and III, of potentials V_1, V_2, and V_3, respectively. We have the general differential equation:

$$
\begin{aligned}
\psi'' + k_i^2 &= 0 \\
k_1 &= \sqrt{\frac{2m}{\hbar^2}(V_1 - E)} \\
k_2 &= \sqrt{\frac{2m}{\hbar^2}(V_2 - E)} \\
k_3 &= \sqrt{\frac{2m}{\hbar^2}(V_3 - E)}
\end{aligned}
$$

This gives us the solutions in each region:

$$
\begin{aligned}
\psi_I &= e^{ik_1 x} + re^{-ik_1 x} \\
\psi_{II} &= Ae^{k_2 x} + Be^{-k_2 x} \\
\psi_{III} &= te^{ik_3 L/2}
\end{aligned}
$$

(b) What boundary conditions must be satisfied?

We must have the following boundary conditions satisfied for the continuity and differentiability:

$$
\begin{aligned}
\psi_I(-L/2) &= \psi_{II}(-L/2) \\
\psi'_I(-L/2) &= \psi'_{II}(-L/2) \\
\psi_{II}(L/2) &= \psi_{III}(L/2) \\
\psi'_{II}(L/2) &= \psi'_{III}(L/2)
\end{aligned}
$$

(c) Calculate the transmission coefficient of the barrier.

Applying the boundary conditions:

$$
\begin{aligned}
e^{-ik_1 L/2} + re^{ik_1 L/2} &= Ae^{k_2 L/2} + Be^{k_2 L/2} \\
-ik_1 e^{-ik_1 L/2} + rik_1 e^{ik_1 L/2} &= k_2 Ae^{-k_2 L/2} - k_2 Be^{k_2 L/2} \\
Ae^{k_2 L/2} + Be^{-k_2 L/2} &= te^{ik_3 L/2} \\
k_2 Ae^{k_2 L/2} - k_2 Be^{-k_2 L/2} &= tik_3 e^{ik_3 L/2}
\end{aligned}
$$

This system gives a transmission coefficient:

$$
\begin{aligned}
T &= |t|^2 \\
&= \left[\frac{k_2 A e^{k_2 L/2} - k_2 B e^{-k_2 L/2}}{ik_3 e^{ik_3 L/2}}\right]^2
\end{aligned}
$$

Where A and B are determined by the boundary conditions.

(d) Where is the particle traveling fastest?

The particle is traveling the fastest in region III where the potential is lowest.

(e) What are the effects of an additional barrier of width w and height V_2 centered at $x = 3L$ while the potential at $x > 3L + w/2$ is the same as V_3? Is the presence of this additional barrier sufficient to permit a bound state and why?

The presence of an additional potential barrier adds another transmission and reflection at either side, which would become a problem near identical to a finite barrier of defined thickness w. The presence of this additional barrier could support a bound state for particular energy $E < V_2$.