Eric Du — Physics 137B

HW 04 — Quantum Mechanics II — February 19, 2023

Collaborators

I worked with **Andrew Binder** to complete this assignment.

Problem 1

Consider a particle of mass m that is free to move in a one-dimensional region of length L that closes on itself (for instance, a bead that slides frictionlessly on a circular wire of circumference L, as in problem 2.46).

a) Show that the stationary states can be written in the form

$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{2\pi i n x/L}, \quad \left(-\frac{L}{2} < x < \frac{L}{2}\right)$$

where $n = 0, \pm 1, \pm 2, \ldots$ and the allowed energies are

$$E_n = \frac{2}{m}\left(\frac{n\pi\hbar}{L}\right)^2$$

Notice that – with the exception of the ground state ($n = 0$) – these are all doubly degenerate.

Solution: This problem is solved in the exact same way 2.46 is solved. Solving the Schrödinger equation, we obtain the solution set:

$$\psi_n(x) = Ae^{ikx} + Be^{-ikx}$$

from the fact that our solutions should be oscillatory, then we now impose the condition that $\psi(x+L) = \psi(x)$, since the bead is circular. Therefore we have:

$$Ae^{ikx}e^{ikL} + Be^{-ikx}e^{-ikL} = Ae^{ikx} + Be^{-ikx}$$

And specifically at $x = 0$, we have:

$$Ae^{ikL} + Be^{-ikL} = A + B$$

And for $x = \pi/2k$, we have:

$$Ae^{ik\pi/2}e^{ikL} + Be^{-ik\pi/2}e^{-ikL} = Ae^{i\pi/2} + Be^{-i\pi/2} \implies Ae^{ikL} - Be^{-ikL} = A - B$$

Adding these two equations at $x = 0$ and $x = \pi/2k$, we get:

$$Ae^{ikL} = A$$

This implies solutions $A = 0$ or $e^{ikL} = 1$. If $A = 0$, then we have:

$$Be^{-ikL} = B \implies kL = 2\pi n$$

and so therefore

$$k = \frac{2\pi n}{L}$$

which works for all n. On the other hand, if $e^{ikL} = 1$, then we get that:

$$kL = 2\pi n \implies k = \frac{2\pi n}{L}$$

which is the same conclusion that we arrived at before. Subtracting the two equations would give us

$$Be^{ikL} = B$$

which we can then solve for a similar relation in terms of A. In either case, the key is that we can set one of them to equal zero, and so our overall wavefunction looks like:

$$\psi_n(x) = \begin{cases} Ae^{\frac{2\pi inx}{L}} & n \geq 0 \\ Be^{\frac{2\pi inx}{L}} & n < 0 \end{cases}$$

after having solved for k. Normalizing this, we get:

$$\int_0^L |\psi_n|^2 dx = A^2 L = B^2 L = 1$$
$$\therefore A = B = \frac{1}{\sqrt{L}}$$

Then, since we can take x to be symmetric about the origin, then we have:

$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{\frac{2\pi inx}{L}}, \quad -\frac{L}{2} < x < \frac{L}{2}$$

which is exactly what we wanted. Furthermore, we can now substitute our expression for ψ into the Schrödinger equation, which would give us:

$$E_n = \frac{2n^2\pi^2\hbar^2}{mL^2} = \frac{2}{m}\left(\frac{n\pi\hbar}{L}\right)^2$$

As desired. □

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b) Now suppose we introduce the perturbation

$$H' = -V_0 e^{-\frac{x^2}{a^2}}$$

where $a \ll L$ (This puts a little "dimple" in the potential at $x = 0$, as though we bent the wire slightly to make a "trap".) Find the first-order correction to E_n, using Equation 7.33. *Hint:* To evaluate the integrals, exploit the fact that $a \ll L$ to extend the limits from $\pm L/2$ to $\pm\infty$; after all, H' is essentially zero outside $-a < x < a$.

Solution: To solve this, we calculate the matrix elements for the degenerate subspace, noticing that for each energy level there is a twofold degeneracy. For the diagonal terms, we have:

$$\langle\psi_n|H'|\psi_n\rangle = \frac{1}{L}\int_{-L/2}^{L/2} -V_0 e^{-x^2/a^2}\, dx = -\frac{V_0}{L}\int_{-\infty}^{\infty} e^{-x^2/a^2}\, dx = -\frac{V_0}{L}a\sqrt{\pi}$$

For the off-diagonal terms, we have:

$$\langle\psi_n|H'|\psi_{-n}\rangle = \frac{1}{L}\int_{-L/2}^{L/2} e^{-2\pi inx/L}(-V_0 e^{-x^2/a^2})e^{-2\pi inx/L}\, dx = -\frac{V_0}{L}\int_{-\infty}^{\infty} e^{-4\pi inx/L} e^{-x^2/a^2}\, dx$$

Plugging this result into an integral calculator, we get:

$$\langle\psi_n|H'|\psi_{-n}\rangle = -\frac{V_0}{L}a\sqrt{\pi}e^{-(2\pi na/L)^2}$$

From here, we have all the matrix elements, all we have to do now is to calculate the eigenvalues of this matrix. Using Equation 7.33, we find that:

$$E_\pm = \frac{1}{2}\left[-\frac{V_0}{L}a\sqrt{\pi} - \frac{V_0}{L}a\sqrt{\pi} \pm \frac{V_0}{L}a\sqrt{\pi}e^{-(2n\pi a/L)^2}\right]$$

Therefore, we get:

$$E_{n+} = -\frac{V_0}{L}a\sqrt{\pi}\left[1 - e^{-(2n\pi a/L)^2}\right]$$
$$E_{n-} = -\frac{V_0}{L}a\sqrt{\pi}\left[1 + e^{-(2n\pi a/L)^2}\right]$$

□

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c) What are the "good" linear combinations of ψ_n and ψ_{-n} for this problem? (*Hint:* use Eq. 7.27). Show that with these states you get the first-order correction using Equation 7.9

Solution: To do this, we just look for the eigenvectors of our perturbed Hamiltonian. Solving Equation 7.27, we obtain:

$$\beta = \alpha \cdot \frac{\frac{-V_0}{L}a\sqrt{\pi}e^{-(2na\pi/L)^2}}{\mp\frac{V_0}{L}a\sqrt{\pi}e^{-(2na\pi/L)^2}} = \mp\alpha$$

And so therefore we get the linear combinations:

$$\overline{\psi}_\pm = \alpha\psi_n \mp \alpha\psi_{-n} = \alpha\frac{1}{\sqrt{L}}\left(e^{2\pi inx/L} \mp e^{-2\pi inx/L}\right)$$

So normalizing this state, we get that $\alpha = \frac{1}{\sqrt{2}}$:

$$\overline{\psi}_+ = \alpha\psi_n - \alpha\psi_{-n} = \frac{1}{\sqrt{2L}}\left(e^{2\pi inx/L} - e^{-2\pi inx/L}\right) = \frac{2i}{\sqrt{2L}}\sin\left(\frac{2\pi nx}{L}\right) = i\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi nx}{L}\right)$$

Likewise for the other state, we get:

$$\overline{\psi}_- = \alpha\psi_n + \alpha\psi_{-n} = \frac{1}{\sqrt{2L}}\left(e^{2\pi inx/L} + e^{2\pi inx/L}\right) = \frac{2}{\sqrt{2L}}\cos\left(\frac{2\pi nx}{L}\right) = \sqrt{\frac{2}{L}}\cos\left(\frac{2\pi nx}{L}\right)$$

To verify that these give the correct perturbation, we calculate:

$$\begin{aligned}
E^1_{n+} &= \langle\overline{\psi}_+|H'|\overline{\psi}_+\rangle \\
&= -\frac{2V_0}{L}\int_{-L/2}^{L/2}\sin^2\left(\frac{2\pi nx}{L}\right)e^{-x^2/a^2}\ dx \\
&\approx -\frac{2V_0}{L}\int_{-\infty}^{\infty}\sin^2\left(\frac{2\pi nx}{L}\right)e^{-x^2/a^2}\ dx
\end{aligned}$$

Plugging this into an integral calculator gives us:

$$E_{n+} = -\frac{2V_0}{L}\cdot\frac{\sqrt{\pi}a\left(1 - e^{-(2\pi na/L)^2}\right)}{2} = -\frac{V_0}{L}a\sqrt{\pi}\left(1 - e^{-(2\pi na/L)^2}\right)$$

And similarly with the other solution:

$$\begin{aligned}
E_{n-} &= -\frac{2V_0}{L}\int_{-\infty}^{\infty}\cos^2\left(\frac{2\ pinx}{L}\right)e^{-x^2/a^2}\ dx \\
&= -\frac{2V_0}{L}\frac{\sqrt{\pi}a\left(e^{-(2\pi na/L)^2}+1\right)}{2} \\
&= -\frac{V_0}{L}a\sqrt{\pi}\left(1+e^{-(2\pi na/L)^2}\right)
\end{aligned}$$

which are the same expressions we got in part (b). □

Problem 2

Suppose we perturb the infinite cubical well (Problem 4.2) by putting a delta function "bump" at the point $(a/4, a/2, 3a/4)$:

$$H' = a^3 V_0 \delta(x - a/4)\delta(y - a/2)\delta(z - 3a/4)$$

Find the first-order corrections to the energy ground state and the (triply degenerate) first excited states.

Solution: The ground state is nondegenerate, so therefore the energy correction is:

$$E_0^1 = \langle 111|H'|111\rangle$$

And so this equals

$$E_0^1 = a^3 V_0 \cdot \left(\frac{2}{a}\right)^3 \sin^2\left(\frac{\pi}{4}\right)\sin^2\left(\frac{\pi}{2}\right)\sin^2\left(\frac{3\pi}{4}\right) = 2V_0$$

after evaluating the integral while using the property that $\int f(x)\delta(x)\,dx = f(0)$. Now we have to calculate the first excited states. First, notice that the states are: $|2,1,1\rangle\;|1,2,1\rangle\,,|1,1,2\rangle$. Now we need to calculate the matrix of the degenerate subspace, and find its eigenvalues. First, we can calculate the diagonal terms:

$$\begin{aligned}
\langle 112|H'|112\rangle &= 8V_0 \sin^2\left(\frac{\pi}{4}\right)\sin^2\left(\frac{\pi}{2}\right)\sin^2\left(\frac{3\pi}{4}\right) = 4V_0 \\
\langle 121|H'|121\rangle &= 8V_0 \sin^2\left(\frac{\pi}{4}\right)\sin^2(\pi)\sin^2\left(\frac{3\pi}{4}\right) = 0 \\
\langle 211|H'|211\rangle &= 8V_0 \sin^2\left(\frac{\pi}{2}\right)\sin^2\left(\frac{\pi}{2}\right)\sin^2\left(\frac{3\pi}{4}\right) = 4V_0
\end{aligned}$$

Now for the off diagonal terms. These aren't too much more tedious, but I will only show one for the sake of brevity:

$$\begin{aligned}
\langle 211|H'|121\rangle &= \left(\frac{2}{a}\right)^3 a^3 V_0 \left[\langle 2|\delta\left(x - \frac{a}{4}\right)|1\rangle\;\langle 1|\delta\left(y - \frac{a}{2}\right)|2\rangle\;\langle 1|\delta\left(z - \frac{3a}{4}\right)|1\rangle\right] \\
&= 8V_0 \left[\sin\left(\frac{\pi}{2}\right)\sin\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{2}\right)\sin\pi\sin^2\left(\frac{3\pi}{4}\right)\right] \\
&= 0
\end{aligned}$$

A very similar process is employed to calculate the other two matrix elements, giving us

$$\begin{aligned}
\langle 211|H'|112\rangle &= -4V_0 \\
\langle 121|H'|112\rangle &= 0
\end{aligned}$$

So now we have a matrix:

$$H' = 4V_0 \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

This gives the eigenvalues $E^1 = 0, 2$ with two solutions for $E = 0$, so therefore the energy correction is $\Delta E = 0, 0, 8V_0$.

$\square$

Problem 3

Use the virial theorem (Problem 4.48) to prove Equation 7.56

Solution: The virial theorem writes:

$$\langle V \rangle = 2E_n$$

And since $V = -\frac{e^2}{4\pi\epsilon_0 r}$ and

$$E_n = -\left(\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right)$$

we can then plug these in:

$$\begin{aligned}
\langle V \rangle &= -\frac{e^2}{4\pi\epsilon_0}\left\langle \frac{1}{r} \right\rangle \\
-2 \cdot \frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{1}{n^2} &= -\frac{e^2}{4\pi\epsilon_0}\left\langle \frac{1}{r} \right\rangle \\
\therefore \left\langle \frac{1}{r} \right\rangle &= \frac{me^2}{4\pi\epsilon_0\hbar^2}\frac{1}{n^2} \\
&= \frac{1}{a_0 n^2}
\end{aligned}$$

which is equation 7.56, as desired. □

Problem 4

Evaluate the following commutators:

a) $[\mathbf{L}\cdot S, \mathbf{L}]$

Solution: To do this we just write out the commutator:

$$\begin{aligned}[\mathbf{L}\cdot\mathbf{S}, L_x] &= [L_xS_x + L_yS_y + L_zS_z, L_x] \\ &= S_x[L_x, L_x] + S_y[L_y, L_x] + S_z[L_z, L_x] \\ &= S_y(-i\hbar L_z) + S_z(i\hbar L_y) \\ &= i\hbar(L_yS_z - L_zS_y) \\ &= i\hbar(\mathbf{L}\times\mathbf{S})_x\end{aligned}$$

The other two components will behave the same way, so combining them gives us all the components summed up altogether:

$$[\mathbf{L}\cdot\mathbf{S}, \mathbf{L}] = i\hbar(\mathbf{L}\times\mathbf{S})$$

□

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b) $[\mathbf{L}\cdot\mathbf{S}, \mathbf{S}]$

Solution: Doing this is much of the same process:

$$\begin{aligned}[\mathbf{L}\cdot\mathbf{S}, S_x] &= [L_xS_x + L_yS_y + L_zS_z, S_x] \\ &= L_x[S_x, S_x] + L_y[S_y, S_x] + L_z[S_z, S_x] \\ &= -L_y(i\hbar S_z) + L_z(i\hbar S_y) \\ &= i\hbar(S_yL_z - S_zL_y) \\ &= \boxed{i\hbar(\mathbf{S}\times\mathbf{L})_x}\end{aligned}$$

And so just like before, combining all three components together we get:

$$\boxed{[\mathbf{L}\cdot\mathbf{S}, \mathbf{S}] = i\hbar(\mathbf{S}\times\mathbf{L})}$$

□

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c) $[\mathbf{L}\cdot\mathbf{S}, \mathbf{J}]$

Solution: Since we have that $\mathbf{J} = \mathbf{L} + \mathbf{S}$, then we have:

$$\begin{aligned}[\mathbf{L}\cdot\mathbf{S}, \mathbf{J}] &= [\mathbf{L}\cdot\mathbf{S}, \mathbf{L}+\mathbf{S}] \\ &= i\hbar(L\times S + S\times L) \\ &= 0\end{aligned}$$

□

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d) $[\mathbf{L}\cdot\mathbf{S}, L^2]$

Solution: Now we can use our previous reuslts. Since we know that $L^2 = L_x^2 + L_y^2 + L_z^2$, and that each of these commutes with L and S, we then have

$$[\mathbf{L}\cdot\mathbf{S}, L^2] = 0$$

□

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e) $[\mathbf{L} \cdot \mathbf{S}, S^2]$

Solution: Using a similar reasoning as the previous problem, we know that $S^2 = S_x^2 + S_y^2 + S_z^2$ and that each of these also commutes with L and S, so:

$$[\mathbf{L} \cdot \mathbf{S}, S^2] = 0$$

$\square$

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f) $[\mathbf{L} \cdot \mathbf{S}, J^2]$

Solution: Since $\mathbf{J} = J_x^2 + J_y^2 + J_z^2 = (L_x + S_x)^2 + (L_y + S_y)^2 + (L_z + S_z)^2$ and $\mathbf{L} \cdot \mathbf{S}$ commutes with both from the previous two parts, then we know that:

$$[\mathbf{L} \cdot \mathbf{S}, J^2] = 0$$

$\square$

Problem 5

How does the threefold degenerate energy

$$E = 3\hbar\omega_0$$

of the two-dimensional harmonic oscillator separate due to the perturbation

$$H' = K'xy?$$

Solution: We know that the energy of a 2D harmonic oscillator can be written as:

$$E = \left(n_x + \frac{1}{2}\right)\hbar\omega + \left(n_y + \frac{1}{2}\right)\hbar\omega = (n_x + n_y + 1)\,\hbar\omega$$

And since we know that the total energy is $E = 3\hbar\omega_0$, then we know that the degenerate states are: $|n_x, n_y\rangle = |0,2\rangle, |1,1\rangle, |2,0\rangle$. So now our goal is to see whether the matrix elements in the degenerate subspace are zero. To do this, we look at whether:

$$K' \langle\psi_n|xy|\psi_n\rangle = 0$$

For all states in the degenerate subspace. Expanding out x and y in terms of raising and lowering operators, we get:

$$\begin{aligned}
K' \langle\psi_n|xy|\psi_n\rangle &= K'\frac{\hbar}{2m\omega_0}\left\langle n_x n_y\middle|(x_+ + x_-)(y_+ + y_-)\middle|n_x' n_y'\right\rangle \\
&= K'\frac{\hbar}{2m\omega_0}\left\langle n_x n_y\middle|x_+y_+ + x_+y_- + x_-y_+x_-y_-\middle|n_x' n_y'\right\rangle \\
&= K'\frac{\hbar}{2m\omega_0}\left(\left\langle n_x n_y\middle|n_{x+1}' n_{y+1}'\right\rangle + \left\langle n_x n_y\middle|n_{x+1}' n_{y-1}'\right\rangle + \left\langle n_x n_y\middle|n_{x-1}' n_{y-1}'\right\rangle + \left\langle n_x n_y\middle|n_{x-1}' n_{y-1}'\right\rangle\right)
\end{aligned}$$

Note here that the only states which will produce a nonzero expectation value are if $|n_x, n_y\rangle = |2,0\rangle$ or $|0,2\rangle$, since if our state is $|1,1\rangle$ then the raising and lowering operators would alter the states so that they are orthogonal to our original one. For the state $|2,0\rangle$ the only term that survives is $\left\langle n_x n_y\middle|n_{x+1}' n_{y-1}\right\rangle$ where $\left|n_x' n_y'\right\rangle = |1,1\rangle$. Therefore, the matrix element is:

$$\langle 2,0|x_+y_-|1,1\rangle = \langle 2,0|\sqrt{2}|2,0\rangle = \sqrt{2}$$

Similarly, we have:

$$\langle 0,2|x_-y_+|1,1\rangle = \langle 0,2|\sqrt{2}|0,2\rangle = \sqrt{2}$$

So we can build our matrix:

$$H' = K'\frac{\hbar}{2m\omega_0}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

which gives us the eigenvalues $\lambda = 0, \pm 2$. So therefore, our threefold degeneracy splits up into three states with $E_0 + 2\Delta E, E_0, E_0 - 2\Delta E$ where

$$\Delta E = K'\frac{\hbar}{2m\omega_0}$$

In other words, our threefold degeneracy splits into three states: one goes up in energy by $2\Delta E$, one stays the same, and the final one goes down in energy by $2\Delta E$. $\square$