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Solution to final exam
FY2045 Quantum Mechanics I
Monday December 7, 2015

Problem 1

a) The wave function curves away from the x axis in the region with zero potential, which means that $E < 0$. In the region with non-zero potential, the wavefunction curves towards the x axis, which means that $E > V_0$.

D $\quad E < 0 \quad V_0 < E$

b) The first excited state in an infinite square well is given by

B $\quad \psi(x) = \sqrt{\frac{2}{L}} \sin(2\pi x/L)$

c) The triangle inequality gives the minimum and maximum values: $|l - s| \leq j \leq l + s$. Since j has to change in integer steps, we get

C $\quad j = \frac{3}{2}, \frac{5}{2}$

d) Calculate $\sigma_x \sigma_y - \sigma_y \sigma_x$ using matrix multiplication, and we find

D $\quad 2i\sigma_z$

e) When $k_B T \ll E_F$, we can set $\mu = E_F$. Calculating $\langle n \rangle$ for $E = E_F$ then gives

B $\quad 1/2$

f) The probabilities are given by the square of the amplitudes (expansion coefficient) of each state.

D $\quad 1/3$

g) The expectation value is given by a weighted average of the possible energies, where the weights are the probabilities (square of the amplitudes). In this case, the possible energy measurements are E_1 and E_3, each with probability 1/2.

C $\quad \frac{5\pi^2\hbar^2}{2mL^2}$

Problem 2

a) The ground state has no zeros, and the first excited state has one zero.

b) Insert the given form of the wave function into the time-independent Schrödinger equation (with $V(x) = 0$ in the well):

$$\begin{aligned} \hat{H}\psi_2(x) &= E_2\psi_2(x) \\ \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_2(x) &= E_2\psi_2(x) \\ \frac{\hbar^2 k_2^2}{2m} &= E_2 \end{aligned}$$

Then we insert $E_2 = V_0 = \hbar^2/(2ma_0^2)$:

$$\begin{aligned} \frac{\hbar^2 k_2^2}{2m} &= \hbar^2/(2ma_0^2) \\ k_2 &= \frac{1}{a_0}. \end{aligned}$$

c) Writing down the time-independent Schrödinger equation for the region $x < 0$, and inserting $E_2 = V_0 = \hbar^2/(2ma_0^2)$, we get:

$$\begin{aligned} \left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + 2V_0\right)\psi_2(x) &= E_2\psi_2(x) \\ \left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + 2\frac{\hbar^2}{2ma_0^2}\right)\psi_2(x) &= \frac{\hbar^2}{2ma_0^2}\psi_2(x) \\ \frac{\partial^2}{\partial x^2}\psi_2(x) &= \frac{1}{a_0^2}\psi_2(x) \end{aligned}$$

This equation has the general solution

$$\psi_2(x) = C\mathrm{e}^{\kappa x} + D\mathrm{e}^{-\kappa x}.$$

We know that the wave function has to go to zero at $-\infty$, since $E_2 < 2V_0$, hence we can set $D = 0$. Inserting this into the Schrödinger equation, we find

$$\begin{aligned}\frac{\partial^2}{\partial x^2} e^{\kappa x} &= \frac{1}{a_0^2} e^{\kappa x} \\ \kappa^2 &= \frac{1}{a_0^2} \\ \kappa &= \frac{1}{a_0}\end{aligned}$$

In a similar manner, using $V(x) = 4V_0$ for $x > L$, we find

$$\kappa' = \frac{\sqrt{3}}{a_0}$$

d) Inserting $x = 0$, and using the continuity of the wave function, we get

$$C = A \sin(-k_2 a).$$

Inserting $x = 0$, and using the continuity of the derivative of the wave function, we get

$$\kappa C = k_2 A \cos(-k_2 a).$$

Dividing the first of these equations by the second, and using that $\kappa = k_2 = \frac{1}{a_0}$, we find

$$\begin{aligned}\tan(-k_2 a) &= 1 \\ k_2 a &= \frac{3\pi}{4}.\end{aligned}$$

Strictly speaking, we can only say that $k_2 a = 3\pi/4 + n\pi$, where n is an integer, but this makes no difference to the wave function, since $\sin(x + n\pi) = \sin(x)$.

To find the width of the well, we use the continuity of the wave function, and the derivative of the wave function, at $x = L$. By dividing the equations like we did above, and using $k_2 = 1/a_0$ and $\kappa' = \sqrt{3}/a_0$, we get

$$\begin{aligned}\frac{1}{k_2} \tan(k_2(L - a)) &= -\frac{1}{\kappa'} \\ \tan(k_2(L - a)) &= -\frac{1}{\sqrt{3}} \\ k_2(L - a) &= \frac{5\pi}{6}.\end{aligned}$$

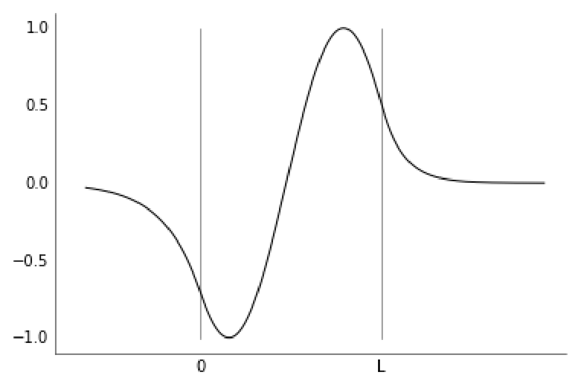
Since we already found that $k_2 a = 3\pi/4$, we have

$$k_2 L = \frac{5\pi}{6} + \frac{3\pi}{4}$$
$$k_2 L = \frac{19\pi}{12}.$$

Again, we can only really say that $k_2 L = \frac{19\pi}{12} + n\pi$, however we can conclude that the length of the well has to be such that the first excited state can have a zero, and still go towards the x-axis at each end in order for the derivative of the wave function to be contiuous everywhere. Hence, $k_2 L$ has to be between π and 2π, and we conclude that the correct value is

$$L = \frac{19\pi}{12} a_0.$$

e) This sketch is made by setting $A = 1$, and then choosing C to match at the boundaries, which means that this is not a correctly normalised wave function.



f) Inserting the given form of the wave function into the expression for the probability current density, we get

$$j(x) = \mathrm{Re}\left\{ \left(\mathrm{e}^{-ikx} + r^* \mathrm{e}^{ikx}\right) \frac{\hbar}{\mathrm{i}m} \frac{\partial}{\partial x} \left(\mathrm{e}^{ikx} + \mathrm{e}^{-ikx}\right) \right\}$$
$$j(x) = \frac{\hbar k}{m} \mathrm{Re}\left\{1 - r\mathrm{e}^{-2\mathrm{i}kx} + r^* \mathrm{e}^{2\mathrm{i}kx} - |r|^2\right\}$$
$$j(x) = \frac{\hbar k}{m} \left(1 - |r|^2\right).$$

In the last step, we have used that $\mathrm{Re}\{a - a^*\} = 0$.

In the region $x > L$, the wave function has to fall off exponentially with increasing x when $E < 4V_0$, since this is a classically forbidden area. Hence, it has to have the form

$$\psi(x) = Ce^{-\kappa x},$$

where κ is a real number. Inserting this into the expression for the probability current density, we find

$$j(x) = \mathrm{Re}\left\{ \mathrm{e}^{-\kappa x} \frac{\hbar}{im} \frac{\partial}{\partial x} \mathrm{e}^{-\kappa x} \right\},$$

and since the expression in the brackets is purely imaginary, we have

$$j(x) = 0.$$

Problem 3

a) First, we find the general expression for the energy eigenstates from the time independent Schrödinger equation

$$\begin{aligned} -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{x}) &= \frac{\hbar^2 \pi^2}{2mL^2} \left(n_x^2 + n_y^2 + n_z^2 \right) \psi(\mathbf{x}) \\ E_{n_x n_y n_z} &= \frac{\hbar^2 \pi^2}{2mL^2} \left(n_x^2 + n_y^2 + n_z^2 \right) \end{aligned}$$

Then, we insert $n_x = 2$, $n_y = 1$, $n_z = 1$, and get

$$E_{211} = 3 \frac{\hbar^2 \pi^2}{mL^2}$$

b) First, we note that the expression for the energy with $L_x \neq L$ becomes

$$E = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2 + n_z^2}{L^2} \right).$$

If we increase the volume of the box, by changing L_x by the infinitesimal amount $\mathrm{d}L_x$, the particle does work on the side of the box, and the energy of the particle changes by an amount

$$\mathrm{d}E = -F \mathrm{d}L_x.$$

Hence

$$\begin{aligned} F &= -\frac{\mathrm{d}E}{\mathrm{d}L_x} \\ &= \frac{\hbar^2\pi^2 n_x^2}{mL_x^3}. \end{aligned}$$

Since pressure is force divided by area, the pressure becomes

$$p = \frac{\hbar^2\pi^2 n_x^2}{mL_x^5},$$

or, since we are evaluating the expression at $L_x = L$, and with $n_x = 1$,

$$p = \frac{\hbar^2\pi^2}{mL^5}.$$

c) We can fit two particles in each spatial state, since they can have opposite spin. Hence, we need to identify the four states with the lowest energy. For a cubic box, these states are $\psi_{111}(x)$, $\psi_{211}(x)$, $\psi_{121}(x)$ and $\psi_{112}(x)$, and the total energy becomes the sum of the energies of the eight particles. We find

$$\begin{aligned} E_{tot} &= \frac{\hbar^2\pi^2}{m}\left[\left(\frac{1^2}{L_x^2} + \frac{1^2+1^2}{L^2}\right) + \left(\frac{2^2}{L_x^2} + \frac{1^2+1^2}{L^2}\right)\right. \\ &\quad \left. + \left(\frac{1^2}{L_x^2} + \frac{2^2+1^2}{L^2}\right) + \left(\frac{1^2}{L_x^2} + \frac{1^2+2^2}{L^2}\right)\right] \\ &= \frac{\hbar^2\pi^2}{m}\left[\frac{7}{L_x^2} + \frac{14}{L^2}\right]. \end{aligned}$$

Then we can calculate the pressure by the same procedure that was used in the previous problem, and we find

$$p = \frac{14\hbar^2\pi^2}{mL^5}.$$

Note that the force only depends on the terms in the expression for the energy which contains L_x, which means we could also write down just those terms. And, note that in this case, with a cubic box and one “excitation” along each axis, the pressure is equal in all directions.

Problem 4

a)

$$
\begin{aligned}
&(H_0 + \lambda\delta(x - L/2))\left(|n\rangle + \lambda|\psi_n^{(1)}\rangle + \mathcal{O}(\lambda^2)\right) \\
&= \left(E_n^0 + \lambda E_n^{(1)} + \mathcal{O}(\lambda^2)\right)\left(|n\rangle + \lambda|\psi_n^{(1)}\rangle + \mathcal{O}(\lambda^2)\right)
\end{aligned}
$$

Multiplying and collecting terms on the left hand side, we get

$$(H_0 - E_n^0)|n\rangle + \lambda(H_0 - E_n^0)|\psi_n^{(1)}\rangle + \lambda\left(\delta(x - L/2) - E_n^{(1)}\right)|n\rangle + (O)(\lambda^2) = 0$$

Separating out the zero order and first order terms, we then find

$$\left(H_0 - E_n^0\right)|n\rangle = 0,$$

$$\left(H_0 - E_n^0\right)\left|\psi_n^{(1)}\right\rangle + \left(\delta(x - L/2) - E_n^{(1)}\right)|n\rangle = 0.$$

or

$$\left(H_0 - E_n^0\right)\left|\psi_n^0\right\rangle = 0,$$

$$\left(H_0 - E_n^0\right)\left|\psi_n^{(1)}\right\rangle + \left(\delta(x - L/2) - E_n^{(1)}\right)\left|\psi_n^0\right\rangle = 0.$$

b) Multiplying the first order equation by $\langle n|$ from the left, we find

$$\langle n|\left(H_0 - E_n^0\right)\left|\psi_n^{(1)}\right\rangle + \langle n|\left(\delta(x - L/2) - E_n^{(1)}\right)|n\rangle = 0.$$

Using that $\langle n|H_0 = \langle n|E_n^0$, the first term becomes 0, and we are left with

$$\langle n|\left(\delta(x - L/2) - E_n^{(1)}\right)|n\rangle.$$

Moving $E_n^{(1)}$ outside of the bracket, and using that $\langle n|m\rangle = \delta_{nm}$, we end up with

$$\lambda E_n^{(1)} = \langle n|\lambda\delta(x - L/2)|n\rangle.$$

c)

$$
\begin{aligned}
\lambda E_1^{(1)} &= \langle 1|\lambda\delta(x - L/2)|1\rangle \\
&= \lambda\frac{2}{L}\int_0^L \sin\frac{\pi x}{L}\delta(x - L/2)\sin\frac{\pi x}{L}\mathrm{d}x \\
&= \lambda\frac{2}{L}\sin^2\frac{\pi}{2} \\
&= \lambda\frac{2}{L}
\end{aligned}
$$

d) The first excited state, and all other states where n is an even number, have a zero at $x = L/2$. Consequently, the particle has zero probability of being at the location of the delta function perturbation, which means that it is unaffected by the perturbation. Hence, the energy corrections are zero.