

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 $E < 0 \quad V_0 < E$

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

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

- 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 $j = \frac{3}{2}, \frac{5}{2}$

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

D $2i\sigma_z$

- 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 $1/2$

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

D $1/3$

- 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 $\frac{5\pi^2 \hbar^2}{2mL^2}$

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

$$\psi_2(x) = Ce^{\kappa x} + De^{-\kappa x}.$$

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

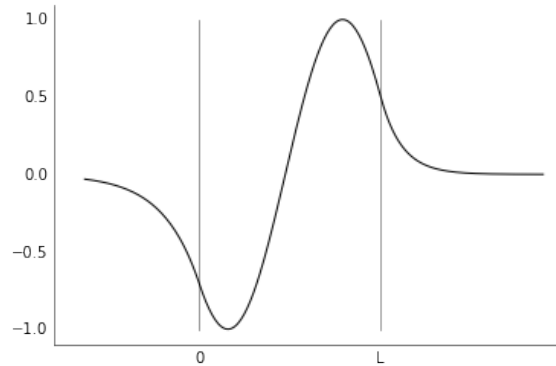
$$k_2 L = \frac{5\pi}{6} + \frac{3\pi}{4}$$

$$k_2 L = \frac{19\pi}{12}.$$

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 continuous 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

$$j(x) = \text{Re} \left\{ (e^{-ikx} + r^* e^{ikx}) \frac{\hbar}{im} \frac{\partial}{\partial x} (e^{ikx} + e^{-ikx}) \right\}$$

$$j(x) = \frac{\hbar k}{m} \text{Re} \{ 1 - r e^{-2ikx} + r^* e^{2ikx} - |r|^2 \}$$

$$j(x) = \frac{\hbar k}{m} (1 - |r|^2).$$

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

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

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

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

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{x}) = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2) \psi(\mathbf{x})$$

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2)$$

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 dL_x , the particle does work on the side of the box, and the energy of the particle changes by an amount

$$dE = -F dL_x.$$

Hence

$$\begin{aligned} F &= -\frac{dE}{dL_x} \\ &= \frac{\hbar^2 \pi^2 n_x^2}{m L_x^3}. \end{aligned}$$

Since pressure is force divided by area, the pressure becomes

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

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

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

- 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

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

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)

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

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

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

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

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

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

or

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

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

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

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

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

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

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)

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

- 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.