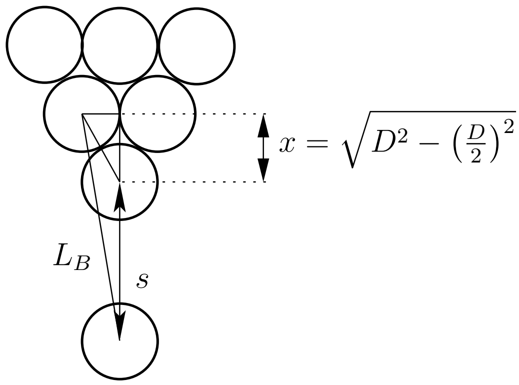
PC2232: Tutorial 7 solutions

Question 1: Scanning tunneling microscope

Let L_B be the distance from atom B to the tip. This can be determined using the geometry drawn below:



From the diagram, we can calculate $x = \sqrt{D^2 - (D/2)^2} = 4.33 \times 10^{-10}$ m. Also,

$$L_B = \sqrt{(s+x)^2 + \left(\frac{D}{2}\right)^2} = 2.446 \times 10^{-9} \text{ m.} \tag{1}$$

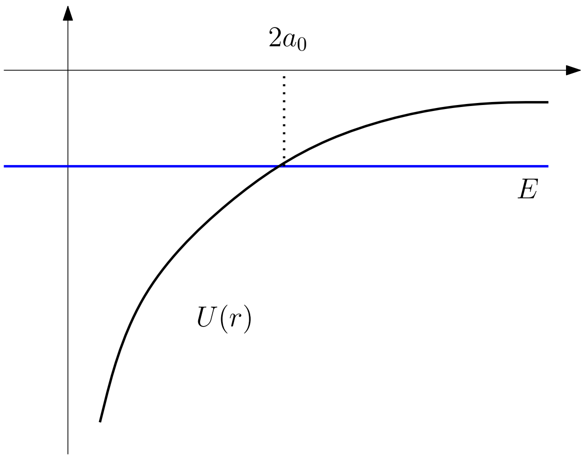
Using $I = I_0 \mathrm{e}^{-2ks}$,

$$\begin{aligned} \frac{I_B}{I_A} &= \frac{\cancel{I_0} \mathrm{e}^{-2k\left(2.446\times10^{-9}\right)}}{\cancel{I_0} \mathrm{e}^{-2k(2\times10^{-9})}} \\ &= 0.01158 \sim 1.1. \end{aligned} \tag{2}$$

Question 2: Hydrogen atom

For the hydrogen atom, the potential function, ground state energy, and Bohr radius are given by

$$U(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}, \quad E_1 = -\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2, \quad a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}. \tag{3}$$

(a) 

(b) The furthest classical region accesible to the electron is where $E = U$ (no more kinetic energy!), which is given by

$$-\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}. \tag{4}$$

Solving for r, we obtain

$$r = 2\left(\frac{4\pi\epsilon_0\hbar^2}{me^2}\right) = 2a_0. \tag{5}$$

So to go beyond $r = 2a_0$, this would imply negative kinetic energy, or complex velocity, which is classically impossible.

(c) Given the wave function

$$\psi = \frac{1}{\sqrt{\pi a_0^3}\mathrm{e}^{-r/a_0}}, \quad |\psi|^2 = \frac{1}{\pi a_0^3}\mathrm{e}^{-2r/a_0}, \tag{6}$$

The probability of finding the particle outside $r > 2a_0$ is

$$\begin{aligned}
P(r > 2a_0) &= \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta\ \sin\theta \int_{2a_0}^{\infty} \mathrm{d}r\ r^2\,|\psi|^2 \\
&= \frac{4\cancel{\pi}}{\cancel{\pi} a_0^3}\int_{2a_0}^{\infty} \mathrm{d}r\ r^2 \mathrm{e}^{-2r/a_0} \\
&= \frac{4}{a_0^3}\left[\left(-\frac{a_0}{2}r^2 - \frac{a_0^2}{4}2r - \frac{a_0^3}{8}2\right)\mathrm{e}^{-2r/a_0}\right]_{2a_0}^{\infty} \\
&= 13\mathrm{e}^{-4} = 0.238.
\end{aligned} \tag{7}$$

Question 3: Average angular momentum
Given that

$$L_z = m_l \hbar, \quad L_z^2 = m_l^2 \hbar^2, \tag{8}$$

and the average of L_z^2 is the sum of its allowed values divided by $(2l+1)$,

$$\langle L_z^2 \rangle_{\text{av}} = \frac{\sum_{m_l=-l}^{l} m_l^2 \hbar^2}{2l+1} = \frac{1}{2l+1} \sum_{m_l=-l}^{l} m_l^2 \hbar^2. \tag{9}$$

Since the terms with negative l are the same as those with positive l,

$$\sum_{m_l=-l}^{l} m_l^2 \hbar^2 = 2 \sum_{m_l=0}^{l} m_l^2 \hbar^2, \tag{10}$$

therefore

$$\langle L_z^2 \rangle_{\text{av}} = \frac{2\hbar^2}{2l+1} \sum_{m_l=0}^{l} m_l^2. \tag{11}$$

Also given that since there is no preferred direction, the averages in all three direction should contribute equally to the total angular momentum squared, i.e., $\langle L_z^2 \rangle_{\text{av}} = \langle L_x^2 \rangle_{\text{av}} = \langle L_y^2 \rangle_{\text{av}}$

$$\begin{aligned} L^2 &= \langle L_x^2 \rangle_{\text{av}} + \langle L_y^2 \rangle_{\text{av}} + \langle L_z^2 \rangle_{\text{av}} \\ &= 3\langle L_z^2 \rangle_{\text{av}} \end{aligned} \tag{12}$$

Substitute Eq. (11) into (12):

$$\begin{aligned} \langle L^2 \rangle_{\text{av}} &= \frac{6\hbar^2}{2l+1} \sum_{m_l=0}^{l} m_l^2 = \frac{\cancel{6}\hbar^2}{\cancel{2l+1}} \cdot \frac{1}{\cancel{6}} l\,(l+1)\,\cancel{(2l+1)} \\ &= \hbar^2 l(l+1). \end{aligned} \tag{13}$$

Question 4: Particle in a 3D box
For the square box of equal side lengths $L_x = L_y = L_z = L$, the energy levels are (see notes on 3D Schrödinger equations)

$$E = \frac{\pi^2 \hbar^2}{2mL^2} \left(n_x^2 + n_y^2 + n_z^2 \right). \tag{14}$$

The energy levels are

n_x	n_y	n_z	E	# of particles occupying
1	1	1	$\frac{\pi^2\hbar^2}{2mL^2}(3)$	2
2	1	1		2
1	2	1	$\frac{\pi^2\hbar^2}{2mL^2}(6)$	2
1	1	2		2
1	2	2		2
2	1	2	$\frac{\pi^2\hbar^2}{2mL^2}(9)$	2
2	2	1		2
1	1	3		
1	3	1	$\frac{\pi^2\hbar^2}{2mL^2}(11)$	1
3	1	1		

(a) The lowest possible total energy is the sum of all the energies of all the particles in the system. Therefore we just need to add up the individual energies of all the particles from the table.

$$E_{\text{total}} = \frac{\pi^2\hbar^2}{2mL^2}\left[2\cdot(3) + 2\cdot(3\cdot 6) + 2\cdot(3\cdot 9) + 11\right] = \frac{\pi^2\hbar^2}{2mL^2}(107) \tag{15}$$

(b) The last (15th) particle only occupy the highest energy, $E = \frac{\pi^2\hbar^2}{2mL^2}(11)$, which has three possibilities $(1,1,3)$, $(1,3,1)$ or $(3,1,1)$. All possibilities are equally likely. So we shall list the most likely position of the particle by each possibility for ψ_{n_x,n_y,n_z}. The direction having quantum number 3 has 3 peaks, $\frac{L}{6}, \frac{3L}{6}, \frac{5L}{6}$. While two directions with quantum number 1 has only one peak at $\frac{L}{2}$. The possibilities and corresponding most likely positions are:

$$\begin{aligned}
&\psi_{1,1,3}: \quad x = \tfrac{L}{2} && y = \tfrac{L}{2} && z = \tfrac{L}{6}, \tfrac{3L}{6}, \tfrac{5L}{6}, \\
&\psi_{1,3,1}: \quad x = \tfrac{L}{2} && y = \tfrac{L}{6}, \tfrac{3L}{6}, \tfrac{5L}{6} && z = \tfrac{L}{2}, \\
&\psi_{3,1,1}: \quad x = \tfrac{L}{6}, \tfrac{3L}{6}, \tfrac{5L}{6}, && y = \tfrac{L}{2}, && z = \tfrac{L}{2},
\end{aligned} \tag{16}$$

(c) The occupation number for each energy levels are

$$\begin{aligned}
E_1 &= 2 \text{ particles}, \\
E_2 &= 6 \text{ particles}, \\
E_3 &= 6 \text{ particles}, \\
E_4 &= 1 \text{ particles}.
\end{aligned} \tag{17}$$

Question 5: Degeneracy counting

For spin-1/2 fermions, there are two particles that can occupy a same quantum number. The degeneracy for each energy level is

$$\begin{aligned} E_1 &= 2K, \quad d_1 = 2, \\ E_2 &= 5K, \quad d_2 = 4, \\ E_3 &= 8K, \quad d_3 = 2, \\ E_4 &= 10K, \quad d_4 = 4, \\ E_5 &= 13K, \quad d_5 = 4. \end{aligned} \tag{18}$$

For three particles having a total energy $20K$, the possible configurations are

$$\begin{aligned} W(1,1,0,0,1) &= \binom{2}{1}\binom{4}{1}\binom{2}{0}\binom{4}{0}\binom{4}{1} = 32 \\ W(1,0,1,1,0) &= \binom{2}{1}\binom{4}{0}\binom{2}{1}\binom{4}{1}\binom{4}{0} = 16 \\ W(0,2,0,1,0) &= \binom{2}{0}\binom{4}{2}\binom{2}{0}\binom{4}{1}\binom{4}{0} = 24 \end{aligned} \tag{19}$$

Question 6: Hybrid states

For the $\psi_{2,1,\pm 1}$ state, the wave function given in the lecture notes are

$$\psi_{2,1,\pm 1} = \mp \underbrace{\left(\frac{1}{8a_0\sqrt{\pi a_0^3}}\right)}_{=A} r\mathrm{e}^{-r/2a_0} \sin\theta\, \mathrm{e}^{\pm \mathrm{i}\phi} \tag{20}$$

where the normalization constant is written as A for convenience.

(a) As instructed, the hybrid state is written as the superposition

$$\begin{aligned} \psi_{2,1,+1} + \psi_{2,1,-1} &= A\left[-r\mathrm{e}^{-r/2a_0} \sin\theta\, \mathrm{e}^{\mathrm{i}\phi} + r\mathrm{e}^{-r/2a_0} \sin\theta\, \mathrm{e}^{-\mathrm{i}\phi}\right] \\ &= -A\mathrm{e}^{-r/2a_0} r \sin\theta \left[\mathrm{e}^{\mathrm{i}\phi} - \mathrm{e}^{-\mathrm{i}\phi}\right] \\ &= -2Ar\sin\theta\sin\phi. \end{aligned} \tag{21}$$

The probability density is

$$|\psi_{2,1,+1} + \psi_{2,1,-1}|^2 = 4A^2\mathrm{e}^{-r/a_0} r^2 \sin^2\theta\, \sin^2\phi. \tag{22}$$

(b)
- Energy: The same, since superposition of solutions with the same energy creates a resulting solution with also the same energy. Also the energy levels

depend on n only.

- Radial dependence: same, since in the above calculation, all have the same radial parts $\propto re^{-r/2a_0}$.
- Angular dependence: Clearly different, since we changed a ϕ part from the form $e^{\pm i}$ to a term related to $\sin\phi$.
- Because the state is proportional to $r\sin\theta\sin\phi$; which is the coordinate y in spherical coordinates.

(c) Instead of addition, do the subtraction:

$$\psi_{2,1,+1} + \psi_{2,1,-1} = -2Ar\sin\theta\cos\phi. \tag{23}$$

Then the state is proportional to $r\sin\theta\cos\phi$, which is the coordinate x in spherical coordinates.

Question 7: Orbital angular momentum

(a)

$$\begin{aligned} L &= \sqrt{L_x^2 + L_y^2 + L_z^2} \\ L^2 - L_z^2 &= L_x^2 + L_y^2. \end{aligned} \tag{24}$$

Since

$$L_z = m_l\hbar, \quad L = \hbar\sqrt{l(l+1)}, \tag{25}$$

therefore

$$\sqrt{L_x^2 + L_y^2} = \hbar\sqrt{l(l+1) - m_l^2}. \tag{26}$$

(b) It is the magnitude of the angular momentum component perpendicular to the z-axis. (In other words, the component in the $x - y$ plane.)

(c) From Eq. (26),

- Maximum: $m_l = 0$, $\sqrt{L_x^2 + L_y^2} = \hbar\sqrt{l(l+1)} = L$.
- Minimum: $m_l = \pm l$, $\sqrt{L_x^2 + L_y^2} = \hbar l(l+1) - l^2 = \hbar\sqrt{l}$.