MIDTERM example 1

SI-MKS

Speed of light in free space	$c = 2.99792458 \times 10^{8}\ \mathrm{m\ s^{-1}}$
Planck's constant	$\hbar = 6.5821188926 \times 10^{-16}\ \mathrm{eV\ s}$
	$\hbar = 1.054571596 \times 10^{-34}\ \mathrm{J\ s}$
Electron charge	$e = 1.602176462 \times 10^{-19}\ \mathrm{C}$
Electron mass	$m_0 = 9.10938188 \times 10^{-31}\ \mathrm{kg}$
Neutron mass	$m_n = 1.67492716 \times 10^{-27}\ \mathrm{kg}$
Proton mass	$m_p = 1.67262158 \times 10^{-27}\ \mathrm{kg}$
Boltzmann constant	$k_B = 1.3806503 \times 10^{-23}\ \mathrm{J\ K^{-1}}$
	$k_B = 8.617342 \times 10^{-5}\ \mathrm{eV\ K^{-1}}$
Permittivity of free space	$\varepsilon_0 = 8.8541878 \times 10^{-12}\ \mathrm{F\ m^{-1}}$
Permeability of free space	$\mu_0 = 4\pi \times 10^{-7}\ \mathrm{H\ m^{-1}}$
Speed of light in free space	$c = 1/\sqrt{\varepsilon_0 \mu_0}$
Avagadro's number	$N_A = 6.02214199 \times 10^{23}\ \mathrm{mol^{-1}}$
Bohr radius	$a_B = 0.52917721 \times 10^{-10}\mathrm{m}$

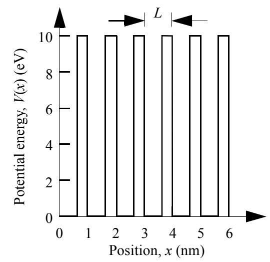
$$a_B = \frac{4\pi\varepsilon_0\hbar^2}{m_0 e^2}$$

Inverse fine-structure constant $\alpha^{-1} = 137.0359976$

$$\alpha^{-1} = \frac{4\pi\varepsilon_0\hbar c}{e^2}$$

Problem 1

An electron moves in the following one-dimensional periodic potential $V(x)$ with $L = 1$ nm ..



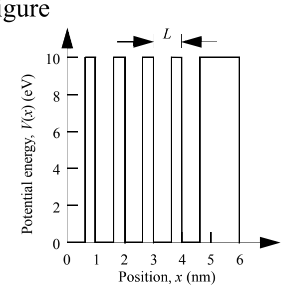
(a) Assuming *periodic boundary conditions* are applied to the potential defined in the region $0 \le x/L < 6$, write down the Hamiltonian for the system and show that the Bloch wave function can be written

$$\psi_k(x+L) = \psi_k(x)e^{ikL}$$

where k is the Bloch wave vector. (20%)

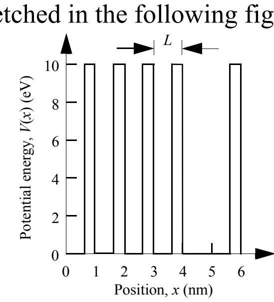
(b) Ignoring electron spin, what is the value of k for the 1^{st} (lowest) energy eigenvalue E_{b1} and what is the value of k for the 2^{nd} energy eigenvalue E_{b2}? Sketch the corresponding wave functions $\psi_{k_1}(x)$ and $\psi_{k_2}(x)$. (20%)

(c) The periodic potential has a missing-atom crystal defect and the new potential is sketched in the following figure



Sketch wave functions $\psi_1(x)$ and $\psi_2(x)$ corresponding to the lowest and next lowest-energy eigenvalues E_{c1} and E_{c2}. Determine if eigenenergy E_{c1} is greater or smaller than E_{b1} in part (b). (40%)

(d) The periodic potential has a crystal defect corresponding to an additional atom and the new potential is sketched in the following figure



Sketch the lowest-energy wave function $\psi_1(x)$ with eigenenergy E_{d1} and state its parity. Determine if eigenenergy E_{d1} is greater or smaller than E_{b1} in part (b). (20%)

Problem 2

An electron is constrained to motion in the x-direction by a potential $V(x) = 0$ for $-\frac{L}{2} < x < \frac{L}{2}$ and $V(x) = \infty$ elsewhere. The electron is in a superposition state consisting of the ground and third excited state such that

$$\psi(x, t) = \frac{1}{\sqrt{2}}(\psi_1(x, t) + \psi_4(x, t))$$

Find explicit analytic expressions for:

(a) The electron probability density, $|\psi(x, t)|^2$. (20%)

(b) The average electron particle position, $\langle x(t) \rangle$. (20%)

(c) The electron current flux,

$$J_x(x, t) = -\frac{ie\hbar}{2m_0}\left(\psi^*(x, t)\frac{\partial}{\partial x}\psi(x, t) - \psi(x, t)\frac{\partial}{\partial x}\psi^*(x, t)\right). \text{ (20\%)}$$

(d) What is the radial frequency and peak value of electron current flux for the case when $L = 10$ nm? (40%)

Problem 3

In classical mechanics, the Hamiltonian for a one-dimensional harmonic oscillator with motion in the x-direction at frequency ω is

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2$$

where m is the mass of the particle and p is the particle momentum.

(a) Introduce operator $\hat{b} = \left(\frac{m_0\omega}{2\hbar}\right)^{1/2}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right)$ and show that in quantum mechanics the Hamiltonian is $\hat{H} = \hbar\omega(\hat{b}^\dagger\hat{b} + 1/2)$. (20%)

(b) Find the normalized wave function for the state $|n = 0\rangle$ defined by $\hat{b}|0\rangle = 0$ and the probability of finding the particle outside the region of classical motion. (30%)

(c) Derive the standard deviation in position Δx and momentum Δp of each harmonic oscillator state $|n\rangle$ and show that they satisfy the Heisenberg uncertainty relation. (20%)

(d) If Δx of an electron mass m_0 in state $|n\rangle$ oscillating at 1 THz is the same as the classical turning point, what is the value of Δp? (30%)

In answering this question, you may wish to use the standard integral $\int_{-\infty}^{\infty} e^{-ax^2}dx = \sqrt{\frac{\pi}{a}}$ and the fact $\frac{1}{\sqrt{\pi}}\int_{|\xi|>1} e^{-\xi^2}d\xi = 0.157$.

Problem 4

(a) An electron moving from left-to-right in the x-direction with energy E encounters a potential step. The potential is $V(x) = V_0$ for $x \geq 0$ and $V(x) = 0$ for $x < 0$. On the left side of the potential step the electron has effective mass m_1 and on the other side it has mass m_2 where $m_2 < m_1$. Calculate the transmission and reflection current in the presence of this potential and discuss any assumptions or approximations you make. (40%)

(b) Sketch the electron wave function $\psi(x)$ when particle energy $E = V_0$ and calculate its contribution to transmission current. (30%)

(c) Sketch the wave function $\psi(x)$ when particle energy $E = \dfrac{V_0}{1 - \dfrac{m_2}{m_1}}$, calculate its contribution to transmission current, and find the *ratio* of electron wavelength either side of $x = 0$. (30%)