MIDTERM example 2

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	$m_\mathrm{n} = 1.67492716 \times 10^{-27}\ \mathrm{kg}$
Proton mass	$m_\mathrm{p} = 1.67262158 \times 10^{-27}\ \mathrm{kg}$
Boltzmann constant	$k_\mathrm{B} = 1.3806503 \times 10^{-23}\ \mathrm{J\ K^{-1}}$
	$k_\mathrm{B} = 8.617342 \times 10^{-5}\ \mathrm{eV\ K^{-1}}$
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	$N_\mathrm{A} = 6.02214199 \times 10^{23}\ \mathrm{mol^{-1}}$
Bohr radius	$a_\mathrm{B} = 0.52917721 \times 10^{-10}\mathrm{m}$

$$a_\mathrm{B} = \frac{4\pi\varepsilon_0\hbar^2}{m_0 e^2}$$

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

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

Problem 1

A one-dimensional crystal with a primitive cell that contains one atom at each lattice site $x_n = nL$, where n is an integer and L is the nearest neighbor atom spacing, has electron wave function $\psi_k(x)$ that can be expressed as a direct lattice sum of single-electron Wannier functions $\phi(x)$ localized around each lattice site x_n.

(a) Show that $\psi_k(x) = \sum_n e^{ikx_n}\phi(x-x_n)$ satisfies the Bloch condition $\psi_k(x+L) = \psi_k(x)e^{ikL}$ for the electron wave function. (40%)

(b) The expectation value of electron energy to first-order is $E_k = \int\psi_k^*(x)\hat{H}\psi_k(x)dx$, where $\hat{H}$ is the Hamiltonian such that $\hat{H}\psi_k(x) = E_k\psi_k(x)$. Assuming little overlap between atomic electron wave functions that are separated by two or more nearest neighbor atom spacings and that the overlap integral $-t = \int\phi^*(x-x_n \pm L)\hat{H}\phi(x-x_n)dx$, find an expression for the electron dispersion relation, $E(k)$, and an expression for the effective electron mass, $m_{\text{eff}}(k)$, in the crystal. (60%)

Problem 2

(a) Derive the current density $\mathbf{J} = -\frac{ie\hbar}{2m}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)$ for a particle mass m and charge e moving in a real potential, $V(x)$. (40%)

(b) If the particle in (a) is moving in a *complex* one-dimensional potential of the form $V = V_1 + iV_2$, where V_1 and V_2 are real constants, show that

$\mathbf{J} = -\frac{ie\hbar}{2m}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right) - \frac{2eV_2}{\hbar}$. (40%)

(c) What physical effect does a positive value of V_2 have on $\mathbf{J}$? If $V_2 = 0$ and $\psi = Be^{-\kappa x - i\omega t}$, where B and κ are real constants, what is the value of $\mathbf{J}$? (20%)

Problem 3
In classical mechanics, the Hamiltonian for a one-dimensional harmonic oscillator with motion in the x-direction at frequency ω is

$$H = \frac{p^2}{2m_0} + \frac{m_0\omega^2}{2}x^2$$

where m_0 is the mass of the particle and p is the particle momentum.

(a) Introduce the operator $\hat{b} = \left(\frac{m_0\omega}{2\hbar}\right)^{1/2}\left(\hat{x} + \frac{i\hat{p}}{m_0\omega}\right)$, find expressions for $\hat{x}$ and $\hat{p}$ in terms of $\hat{b}$ and $\hat{b}^\dagger$, substitute into the Hamiltonian and show that in quantum mechanics $\hat{H} = \hbar\omega(\hat{b}^\dagger\hat{b} + 1/2)$. (20%)

(b) Show that the $n = 0$ ground-state $|0\rangle$ is defined by $\hat{b}|0\rangle = 0$. (20%)

(c) Find the normalized ground-state wave function. (20%)

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

(e) If the standard deviation in momentum is $\Delta p = 5 \times 10^{-25}$ kg m s^{-1}, what is the value of the standard deviation in position for the state $|0\rangle$ and the state $|3\rangle$? (20%)

In answering this question, you may wish to use the standard integral $\int_{-\infty}^{\infty} e^{-ax^2}dx = \sqrt{\frac{\pi}{a}}$.

Problem 4
The first four energy eigenvalues and eigenfunctions for an electron with effective mass $m_e^* = 0.07 \times m_0$ confined to the asymmetric potential well sketched in the following figure and bounded by barriers of infinite energy for $x < 0$ nm and $x > 50$ nm are:
$E_1 = 0.0248$ eV, $E_2 = 0.0973$ eV, $E_3 = 0.2000$ eV, $E_4 = 0.2062$ eV.

(a) Sketch the corresponding wave functions and explain the qualitative differences between each wave function. (50%)

(b) What can you say about the dipole matrix elements $\langle 1|x|3\rangle$ and $\langle 1|x|4\rangle$ for optical transitions? (50%)