MIDTERM example 3

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

Six identical atoms are arranged with equal nearest neighbor spacing in a ring of radius $r = 0.15$ nm.

(a) Using periodic boundary conditions, determine the wave vectors and eigenenergies for free electrons confined to the ring. If each atom contributes a single free electron to the ring, calculate the sum of the ground-state energies of these electrons. (30%)

(b) Repeat part (a) but with the atoms arranged in a linear chain, assuming an infinite potential outside the chain. (30%)

(c) Obtain an estimate of the free-electron contribution to the energy (in eV) required to break the ring of atoms into a linear chain. How is your result modified if the electrons move in a periodic potential due to the presence of the atom ion cores? (40%)

Problem 2

A particle of charge e, mass m, and momentum p oscillates in a one-dimensional harmonic potential $V(x) = m\omega_0^2 x^2/2$ and is subject to an oscillating electric field $|\mathbf{E}|\cos(\omega t)$.

(a) Write down the Hamiltonian of the system. (10%)

(b) Find $\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle$. (30%)

(c) Find $\frac{\mathrm{d}}{\mathrm{d}t}\langle p\rangle$ and show that $\frac{\mathrm{d}}{\mathrm{d}t}\langle p\rangle = -\langle\frac{\mathrm{d}}{\mathrm{d}x}V(x)\rangle$. Under what conditions is the quantum mechanical result $m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle x\rangle = -\langle\frac{\mathrm{d}}{\mathrm{d}x}V(x)\rangle$ the same Newton's second law in which force on a particle is $F = m\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\frac{\mathrm{d}}{\mathrm{d}x}V(x)$? (30%)

(d) Use your results in (b) and (c) to find the time dependence of the expectation value of position $\langle x\rangle(t)$. What happens to the maximum value of $\langle x\rangle$ as a function of time when $\omega_0 = \omega$ and when ω is close in value to ω_0? (30%)

Problem 3

The Hamiltonian of a particle mass m moving in a one-dimensional harmonic oscillator potential can be written

$$H = \hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right)$$

where ω is the angular frequency of oscillation and the operator

$$\hat{b} = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} + \frac{i\hat{p}}{m_0\omega}\right)$$

satisfies the commutation relations $[\hat{b}, \hat{b}^\dagger] = 1$ and $[\hat{b}, \hat{b}] = [\hat{b}^\dagger, \hat{b}^\dagger] = 0$.

(a) Show ground-state wave function $\psi_{n=0} = |0\rangle$ is defined by $\hat{b}|0\rangle = 0$. (30%)

(b) Find the normalized ground-state and first-excited state wave function. (30%)

(c) The operator $\frac{1}{\sqrt{2}}(1 + \hat{b}^\dagger)$ acts on the state $|0\rangle$ and creates a new state $\psi(x, t)$.

Find the probability density $|\psi(x, t)|^2$ and expectation value of position $\langle x(t)\rangle$. (40%)

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

(a) Classically a change in charge density, ρ, is related to divergence of current density, $\mathbf{J}$. Use this fact and the time-dependent Schrödinger wave equation describing the motion of particles of mass *m* and charge *e* in a real potential to derive the probability current $\mathbf{J} = -\frac{ie\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*)$. (40%)

(b) If a wave function in free-space can be expressed as $\psi(x, t) = Ae^{i(kx - \omega t)} + Be^{i(-kx - \omega t)}$ show that particle flux is proportional to $|A|^2 - |B|^2$. (30%)

(c) Calculate the tunnel current associated with an electron wave function of the form $\psi(x, t) = Be^{-\kappa x - \omega t}$ where κ is real. (30%)