QUANTUM MECHANICS—EXAMPLES

Charge on electron: 1.6×10^{-19} C. Mass of electron: 9.1×10^{-31} kg
Mass of proton: 1.67×10^{-27} kg
Planck's constant: $\hbar = 1.05458 \times 10^{-34} Js$; $h = 6.626 \times 10^{-34} Js$

1. **ELECTRONIC SHELL MODEL, BONDING.**
   Look up the periodic table and find the atomic numbers of the elements boron (B), molybdenum (Mo) and gadolinium (Gd). Specify the electronic configurations of the atoms of B, Mo and Gd.

2. Find the atomic numbers of gallium (Ga) and arsenic (As). The bonding of a gallium arsenide, $GaAs$, molecule is said to be 31% ionic and 69% covalent. What do you think that this means?

3. **FREE ELECTRONS**
   Find the Fermi energy ε_F and Fermi velocity v_F of the metals potassium, K, and aluminium, Al, if they are modelled in terms of the free electron model given that their conduction electron number densities are 1.40 $10^{28} m^{-3}$ and 18.1 $10^{28} m^{-3}$ respectively.

4. The total energy of a free electron model of a metal is

$$E_{tot} = \frac{3}{5} N \varepsilon_F = \frac{3}{5} N \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{\frac{2}{3}},$$

   where N is the number of electrons and V the volume of the system. Show that the bulk modulus B (i.e. inverse of the compressibility of this system) is $\frac{2N\varepsilon_F}{3V}$. [Note $B = -V \frac{\partial P}{\partial V}|_N = V \frac{\partial^2 E_{tot}}{\partial V^2}|_N$.]

5. Suppose that free electrons move in two dimensions and that the electron wavefunctions satisfy the periodic boundary conditions

$$\psi(x, y) = \psi(x + L_x, y) = \psi(x, y + L_y).$$

   Show that the plane waves, $\psi = e^{i(k_x x + k_y y)}$ with

$$(k_x, k_y) = \left(\frac{2\pi n_x}{L_x}, \frac{2\pi n_y}{L_y} \right)$$

   where n_x and n_y integers, are allowed eigenfunctions of the free electron Hamiltonian ($H = -(\hbar^2/2m)\nabla^2$).

   Show that all states with energy less than ε lie in a circle in wavenumber space of radius $k = \sqrt{\frac{2m\varepsilon}{\hbar^2}}$ and that their number, N, is given by $N = \frac{A}{2\pi} k^2$, where A is the area of the rectangle with side lengths L_x and L_y.

   Compute the density of states, $n(\varepsilon)$, for this two dimensional system.

6. **PROBABILITY CURRENT IN 3D**
In quantum mechanics consideration of charge conservation leads to this expression for the current in 1D

$$j = \frac{\hbar}{2im}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right).$$

To derive it we start with Schrödinger's equation and use it to obtain an expression for $\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t}$. Charge conservation in 1D means that $\frac{\partial j}{\partial x} = -\frac{\partial \rho}{\partial t}$ so that the corresponding current j can be identified since ρ is the charge density $\psi^*\psi$. (See notes provided). For the 3D case, show that

$$\frac{\partial \rho}{\partial t} = \psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} = -\boldsymbol{\nabla} \cdot \boldsymbol{j}.$$

Hence show that the corresponding current is

$$\boldsymbol{j} = \frac{\hbar}{2im}\left(\psi^* \boldsymbol{\nabla} \psi - \psi \boldsymbol{\nabla} \psi^*\right).$$