QUANTUM MECHANICS
ANSWERS to EXAMPLES

1. **ELECTRONIC SHELL MODEL, BONDING**
   Boron, B, has an atomic number of 5 and electronic configuration

   $$1s^2\,2s^2 2p^1.$$

   Molybdenum, Mo, has $Z = 42$ and configuration

   $$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6\,4d^5 5s^1.$$

   Gadolinium, Gd, has $Z = 64$ and configuration

   $$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6\,4f^7 5d^1 6s^2.$$

2. Gallium (31) and arsenic (33) are either side of germanium (32) in the periodic table. The structure of GaAs might therefore be expected to be similar to that of Ge which would be purely covalent with four electrons involved in the bonding. However, Ga has a nuclear charge of 1 less than that of Ge and As has a nuclear charge of 1 more. As a result there will tend to be a net transfer of electrons to As from the Ga (the As nuclear charge is more attractive). If the bonding is 31% ionic, you would expect to find that the net charge on the Ga and As atoms were $+.31 \times 3e$ and $-.31 \times 3e$ respectively. (If the bond were fully ionic three electrons would transfer to the As to fill its shell and empty the Ga shell.)

3. **FREE ELECTRONS**
   The Fermi energy $\varepsilon_F = \frac{\hbar^2}{2m}(3\pi^2)^{\frac{2}{3}}\rho^{\frac{2}{3}}$ and Fermi velocity $v_F = \frac{\hbar}{m}(3\pi^2)^{\frac{1}{3}}\rho^{\frac{1}{3}}$ where ρ represents the electron number density. For potassium K the values are $\varepsilon_F = 2.12$ eV and $v_F = 0.86\,10^6$ ms^{-1} and for aluminium Al, $\varepsilon_F = 11.7$ eV and $v_F = 2.03\,10^6$ ms^{-1}.

4. The expression for the bulk modulus B is found from $V\frac{\partial^2 E_{tot}}{\partial V^2}|_N$ by straightforward partial differentiation. Use of the expression for ε_F leads to the required result.

5. The periodicity condition means

   $$e^{ik_x L_x} = 1 \Rightarrow k_x = \frac{2n_x\pi}{L_x} \;\; \text{and} \;\; e^{ik_y L_y} = 1 \Rightarrow k_y = \frac{2n_y\pi}{L_x}.$$

   In addition the functions $e^{i(k_x x + k_y y)}$ are eigenstates of the free electron hamiltonian with eigenvalue $E = \hbar^2(k_x^2 + k_y^2)/2m$.

   Writing $\mathbf{k} = (k_x, k_y)$, all the states with energy less than ε have $|\mathbf{k}|^2 < 2m\varepsilon/\hbar^2$, *ie* lie inside a circle in 'k-space'.

   Now, the separations of allowed k states are $2\pi/L_x$ and $2\pi/L_y$ in the x- and y-directions, so that the area occupied in k-space by one allowed state is $4\pi^2/(L_x L_y) = 4\pi^2/A$. Each of these states can be occupied by an electron with

spin up and spin down, so the number of allowed states with energy less than ε is given by

$$N = \frac{2 \times \text{Area of circle radius } k}{\text{Area for 1 allowed state in k space}} = \frac{A}{2\pi}k^2,$$

or in terms of ε:

$$N = \frac{Am}{\pi\hbar^2}\varepsilon.$$

Note that the rhs has no dimensions as the lhs is a number.

The density of states, $n(\varepsilon)$, is given by:

$$n(\varepsilon)d\varepsilon = \frac{dN}{d\varepsilon}d\varepsilon = \frac{Am}{\pi\hbar^2}d\varepsilon,$$

ie $n(\varepsilon)$ is constant. We now have $n(\varepsilon) \sim \varepsilon^{-1/2}$ in 1D, $n(\varepsilon) \sim \varepsilon^0$ in 2D and $n(\varepsilon) \sim \varepsilon^{1/2}$ in 3D.

6. **PROBABILITY CURRENT IN 3D**

   One needs to write

   $$\psi^*\nabla^2\psi - \psi\nabla^2\psi^* = \boldsymbol{\nabla} \cdot \left(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\right).$$

   to obtain the result.

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