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1. Answer the following ten short questions. Briefly explain your answer (**20 Points**).

(a) Diamond is a fcc structure with a lattice constant (conventional unit cell) of 3.57 Å, calculate the density of diamond.

In one cubic of $(3.57 \text{Å})^3$, there are 8 carbon atoms. Each atom weighs

$$m = 1.67 \times 10^{-27} \times 12 = 20 \times 10^{-27} \text{ kg}$$

$$\rho = \frac{20 \times 10^{-27} \text{ kg} \times 8}{3.57^3 \times 10^{-30} \text{ m}^3} = 3.5 \times 10^3 \text{ kg/m}^3$$

(b) The speed of sound of a one-dimensional monatomic lattice chain of Si atoms with a lattice constant of 5.4 Å is 5000 m/s, estimate the spring constant between two adjacent atoms.

From $\omega = 2\sqrt{\frac{k}{m}} \left| \sin \frac{ka}{2} \right|$

$v = \frac{d\omega}{dk} \approx a\sqrt{\frac{k}{m}}$ for acoustic waves

$$k = \left(\frac{v}{a}\right)^2 m = 28 \times 1.67 \times 10^{-27} \times \left(\frac{5000}{5.4 \times 10^{-10}}\right)^2 = 4 \text{ N/m}$$

(c) Estimate the first energy level of an electron inside a quantum well of width 20 Å with infinite potential barrier height.

$$E_n = \frac{1}{2m}\left(\frac{hn}{2L}\right)^2$$

$n=1$ $$E_1 = \frac{1}{2 \times 9.1 \times 10^{-31}} \left(\frac{6.6 \times 10^{-34}}{2 \times 20 \times 10^{-10}}\right)^2 = 1.5 \times 10^{-20} \text{ J} = 0.094 \text{ eV}$$

(e) The bandgap of a direct-gap semiconductor is 1 eV. What would be the wavelength of a laser made of this semiconductor utilizing photon emission from the conduction band to the valence band?

$$h\nu = 1 \text{ eV}$$

$$h \cdot \frac{c}{\lambda} = 1 \text{ eV}$$

$$\lambda = \frac{hc}{1 \text{ eV}} = \frac{6.6 \times 10^{-34} \times 3 \times 10^8}{1.6 \times 10^{-19}} \text{ m} = 1.24 \text{ μm}$$

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2 (**20 Points**).

Treat oxygen as an ideal gas. Estimate its thermal conductivity at 800 K and 1 atm. To answer this question, you need also to estimate the following:

(a) Average thermal velocity of the oxygen atoms.
(b) Specific heat of oxygen.
(c) Mean free path (taking the effective diameter of the O_2 molecule as 2.0 Å).

(a) Average thermal velocity is

$$\frac{1}{2}mv^2 = \frac{3}{2}k_BT$$

$$v = \sqrt{\frac{3k_BT}{m}} = \sqrt{\frac{3\times1.38\times10^{-23}\times800}{32\times1.67\times10^{-27}}} = 787 \text{ m/s}$$

(b) Oxygen has 3 degrees of translational freedom and 2 degrees of rotational freedom. Each degree of freedom contributes $\frac{1}{2}k_BT$. Specific heat is

$$C = \frac{5}{2}R = \frac{5}{2}\times 8.314 \text{ J/K}\cdot\text{mol} = 20.788 \text{ KJ/K}\cdot\text{kmol}$$

$$= 20.788/32 \ \frac{\text{KJ}}{\text{Kg}}\text{/K} = 649.6 \text{ J/Kg}\cdot\text{K}$$

(c)

$$\Lambda = \frac{k_BT}{\pi P D^2} = \frac{1.38\times10^{-23}\times800}{\pi\times1.01\times10^{5}\times(2\times10^{-10})^2} = 8.7\times10^{-7} \text{ m}$$

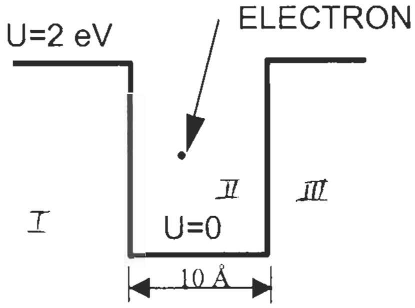
$$\rho = \frac{P}{RT} = \frac{1.01\times10^5}{8.314/32\times10^3\times800} = 0.434 \text{ kg/m}^3$$

$$k = \frac{1}{3}Cv\Lambda = \frac{1}{3}\times649.6\times0.434\times787\times8.7\times10^{-7}$$

$$= 0.064 \text{ W/mK}$$

3. (**20 Points**).

Determine the energy levels of an electron in a finite barrier height potential well as shown in the following figure.



Solution: The solution of the Schrödinger equation for I, II, III are

I: $\psi_I(x) = A e^{+k_I x}$ where $k_I = \sqrt{\frac{2m(U-E)}{\hbar^2}}$

II: $\psi_{II}(x) = B e^{ik_{II}x} + C e^{-ik_{II}x}$ where $k_{II} = \sqrt{\frac{2mE}{\hbar^2}}$

III: $\psi_{III} = D e^{k_I(x-L)}$

Continuity requirements gives

$$A = B + C$$

$$k_I A = i k_{II} (B - C)$$

$$B e^{ik_{II}L} + C e^{-ik_{II}L} = D$$

$$ik_{II}(B e^{ik_{II}L} - C e^{-ik_{II}L}) = k_I D$$

The equations have solutions only when

$$\begin{vmatrix} 1 & -1 & -1 & 0 \\ k_I & -ik_{II} & ik_{II} & 0 \\ & e^{ik_{II}L} & e^{-ik_{II}L} & -1 \\ & ik_{II}e^{ik_{II}L} & -ik_{II}e^{-ik_{II}L} & -k_I \end{vmatrix} = 0$$

Solving this eigenvalue equation leads to allowable energy levels E.

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4. **(20 Points)**

The energy dispersion relation of a bulk semiconductor is

$$E - E_c = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_{11}} + \frac{k_y^2}{m_{22}} + \frac{k_z^2}{m_{33}}\right)$$

Derive an expression for the density of states per unit volume.

Solution: The constant energy surface is an ellipsoid. The volume of constant energy surface in k-space is

$$V = \frac{4}{3}\pi\sqrt{\frac{2m_{11}E'}{\hbar^2}}\sqrt{\frac{2m_{22}E'}{\hbar^2}}\sqrt{\frac{2m_{33}E'}{\hbar^2}}$$

$$= \frac{4\pi}{3}\frac{(2E')^{\frac{3}{2}}(m_{11}m_{22}m_{33})^{\frac{1}{2}}}{\hbar^3} \qquad \text{where } E' = E - E_c$$

Between E to E+dE, the number of states is

$$\frac{\overset{\text{volume of space in k-space}}{dV}}{\underset{\text{volume of one state in k space}}{\left(\frac{2\pi}{L}\right)^3}} \times \underset{\text{spin}}{2}$$

$$D(E) = \frac{1}{V}\frac{2V dV}{8\pi^3 dE} = \frac{1}{4\pi^3}\cdot\frac{4\pi}{3}\times\frac{3}{2}\times 2\sqrt{E}\,\frac{(m_{11}m_{22}m_{33})^{\frac{1}{2}}}{\hbar^3}$$

$$= \frac{(2m_{11}m_{22}m_{33})^{\frac{1}{2}}\sqrt{E-E_c}}{\pi^2\hbar^3}$$

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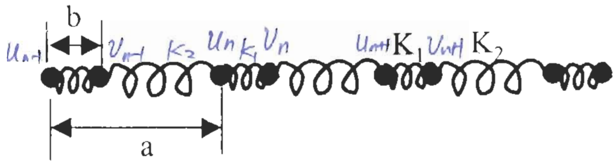
5. (**20 Points**)

Consider a diatomic chain of atoms as shown in the following figure. The distance between the two atoms per lattice point is b and the lattice constant is a. The masses of the two atoms are identical but the spring constants between them are different. Derive an expression for the phonon dispersion in such a diatomic lattice chain.



Solution: Use u_i to denote the displacement of one-type of atom and v_i to denote the displacement of the other type as shown. The Newton's 2nd law is

$$m\frac{d^2u_n}{dt^2} = K_1(v_n - u_n) - K_2(u_n - v_{n-1})$$

$$m\frac{dv_n}{dt^2} = K_2(u_{n+1} - v_n) - K_1(v_n - u_n)$$

I will try the solutions of the following form

$$u_n = u_0 \exp[-i(\omega t - nak)]$$

$$v_n = v_0 \exp[-i(\omega t - nak)]$$

We get

$$-m\omega^2 u_0 = k_1[v_0 - u_0] - k_2[u_0 - v_0 e^{-ika}]$$

$$-m\omega^2 v_0 = k_2[u_0 e^{ika} - v_0] - k_1[v_0 - u_0]$$

So

$$[(k_1+k_2) - m\omega^2]u_0 - [k_1 + k_2 e^{-ika}]v_0 = 0$$

$$[k_1 + k_2 e^{ika}]u_0 - [k_1 + k_2 - m\omega^2]v_0 = 0$$

Solving the eigen value, we get

$$\omega^2 = \frac{(k_1+k_2) \pm \sqrt{k_1^2 + k_2^2 + 2k_1k_2\cos ka}}{M}$$