

Quiz#2, Solution Key

(1) (a) The *Planck* function that describes it is $\langle n_k \rangle = \frac{1}{\exp[\hbar\omega(k)/k_B T] - 1} = \langle n_\omega \rangle$.

(b) Number of lattice-wave states between 0 and k in k space = $N(k)$

$N(k) = V/(2\pi)^3 * (4/3)\pi k^3$ where V is the real-space volume of the sample. By the chain rule of calculus, $D(\omega) = dN/d\omega = (dN/dk)(dk/d\omega)$ and $dN/dk = V/(2\pi)^3 * 4\pi k^2 = (V/2\pi^2) (\omega/v)^2$; $dk/d\omega = 1/v$; both according to Debye model. So $D(\omega) = (V/2\pi^2)\omega^2/v^3$

(c) Total energy is $U = 3 \cdot \int_0^{\omega_D} \langle n_\omega \rangle \cdot D(\omega) \cdot d\omega$ or $U = \frac{3V}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\hbar\omega^3}{\exp[\hbar\omega(k)/k_B T] - 1} d\omega$

where the factor of 3 is for the number of acoustical modes (one longitudinal, two transverse) and ω_D is the maximum frequency of the Debye model. This is defined by noting that each primitive cell contributes one k state in the first Brillouin zone, so that

$$N_C = \int_0^{\omega_D} D(\omega) d\omega = (V/6\pi^2 v^3) \omega_D^3 = (V/6\pi^2 v^3) \omega_D^3 \text{ or } \omega_D = (6\pi^2 N_C/V)^{1/3} \cdot v.$$

(d) At high temperatures, we can approximate the Planck function by $\frac{1}{\exp[\hbar\omega/k_B T] - 1} \approx \frac{k_B T}{\hbar\omega}$, so

we can approximate $U \approx \frac{3V}{2\pi^2 v^3} \int_0^{\omega_D} k_B T \cdot \omega^2 d\omega = \frac{V \cdot k_B T}{2\pi^2 v^3} \omega_D^3$. According to the definition of

ω_D in (c), this becomes $U = 3N_C k_B T$. So the heat capacity is given by $C \approx dU/dT = 3N_C k_B$.

2.(a) In 2D, $N(k) = (L/2\pi)^2 \pi k^2 = Ak^2/(4\pi)$. So $D(U) = dN/dU = (dN/dk)(dk/dU) = (Ak/2\pi)(m/\hbar^2 k) =$

$(mA/2\pi\hbar^2)$. So the sheet density $\sigma_S = A^{-1} \int_0^{\infty} f_{FD} D(U) dU = \int_0^{\infty} \frac{2(m/2\pi\hbar^2) dU}{\exp[(U - U_F)/k_B T] + 1}$ where the

factor of 2 is for spin.

(b). In the low temperature limit, we treat f_{FD} as a step function to get

$$\sigma_S \approx \int_0^{U_{F0}} 2(m/2\pi\hbar^2) dU = mU_{F0}/\pi\hbar^2 \text{ or } U_{F0} = \pi\hbar^2 \sigma_S / m. \text{ For the stated sheet density, and GaAs } (m^* = 0.067m_e), U_{F0} = 5.7 \times 10^{-21} \text{ J} = 36 \text{ meV}.$$

(c) The Fermi velocity is related to U_{F0} by $v_F = (2U_{F0}/m)^{1/2}$. Similarly, the Fermi temperature is given by $T_F = U_{F0}/k_B$. For the given U_{F0} and $m = m^*$ (GaAs), we get $v_F = 4.3 \times 10^5 \text{ m/s}$ and $T_F = 413 \text{ K}$.

3. (a) k is the crystal wavevector. $\hbar k$ is not an eigenvalue of the canonical momentum operator. In the relationship between U and k , there are in principle an infinite number of solutions for each k , indexed by the integer n . For each n , the solution U vs k is called an *energy band*.

$$(b) \psi(x) = \sum_k C_k e^{jkx} \quad V(x) = \sum_G V_G e^{jGx}$$

(c) For one Fourier coefficient in expansion of $V(x)$, the bandgap at Bragg plane is: $U_G = 2V_G$

4. (a) The expression $U(\vec{k}) = \theta(U - U_0) \left\{ U_0 + \frac{\hbar^2}{2} [\alpha(k_x - k_{0x})^2 + \beta(k_y - k_{0y})^2 + \gamma(k_z - k_{0z})^2] \right\}$ represents an

ellipsoid if $\alpha \neq \beta \neq \gamma$, and a spheroid if any two of α , β , and γ are equal. If $\alpha = \beta = \gamma$, the constant-energy surface is a sphere.

(b) $\vec{v}_g = \hbar^{-1} \vec{\nabla}_k U_n(\vec{k})$, which has components $v_{gx} = 0$, $v_{gy} = 0$, and $v_{gz} = 0$ at $\vec{k} = \vec{k}_0$

(c) The effective mass is defined by $m^* = \hbar^2 \left(\frac{\partial^2 U}{\partial k^2} \right)^{-1}$, which yields $m_{xx} = 1/\alpha$, $m_{yy} = 1/\beta$, and $m_{zz} = 1/\gamma$.