

Final Exam Solution Key: 17 March 2008**(1) Thermodynamics and Stat Mech**

(a)  $U = -\mathbf{p} \cdot \mathbf{E}$  where  $\mathbf{p}$  points from  $-$  to  $+$  charge and has magnitude  $qd$ ,  $q = e$  (one electron) and  $d = a/2$ .

So for  $\mathbf{E}$  as shown along the  $x$  axis, the potential energy of the two states is  $U_1 = -\mathbf{p}_1 \cdot \mathbf{E} = ea/2$ , and (since  $\mathbf{p}_1$  and  $\mathbf{E}$  are antiparallel) and  $U_2 = -\mathbf{p}_2 \cdot \mathbf{E} = -ea/2$  (since  $\mathbf{p}_2$  and  $\mathbf{E}$  are parallel)

By assuming Boltzmann statistics, we can thus write probability of occupancy of the *both dipole*

$$\text{states as } f_i = C e^{-U_i/k_B T} \quad \text{where} \quad C = \left( \sum_{i=1}^4 e^{-U_i/k_B T} \right)^{-1} \quad \text{is the normalization constant.}$$

$$\text{So: Dipole (1) } f_1 = C e^{-U_1/k_B T} = C e^{(-eaE/2k_B T)}; \quad \text{Dipole (2): } f_2 = C e^{-U_2/k_B T} = C e^{(eaE/2k_B T)}$$

$$C = \{ \exp[eaE/(2k_B T)] + \exp[-eaE/(2k_B T)] \}^{-1}$$

(b) Substitution of  $a = 3 \times 10^{-10}$  m,  $E = 1 \times 10^8$  V/m, and  $T = 300$  K yields  $eaE/(2k_B T) = 0.58$ , so

$$C = [\exp(0.29) + \exp(-0.29)]^{-1} = [1.786 + 0.56]^{-1} = 0.426, \text{ and we get: } \mathbf{f}_1 = \mathbf{0.24}, \mathbf{f}_2 = \mathbf{0.76}$$

(c) From statistics,  $\langle \vec{\mathbf{p}} \rangle = \sum_i \vec{\mathbf{p}}_i \cdot \mathbf{f}_i = 0.24 \cdot (ea/2)(-\vec{\mathbf{x}}) + 0.76 \cdot (ea/2)(\vec{\mathbf{x}}) = 0.52(ea/2)\vec{\mathbf{x}}$

(d) Substitution:  $\langle \vec{\mathbf{p}} \rangle = 1.25 \times 10^{-29} \vec{\mathbf{x}}$  [Cb-m], and  $\vec{\mathbf{P}} = \rho \langle \vec{\mathbf{p}} \rangle = 1.25 \times 10^{-7} \vec{\mathbf{x}}$  Cb/m<sup>2</sup> since  $\rho = 10^{22}/\text{m}^3$

(e)  $\chi_E = (\epsilon_0^{-1}) \frac{\partial \mathbf{P}}{\partial E} = (\rho / \epsilon_0) (\partial / \partial E) | \sum_i \vec{\mathbf{p}}_i \cdot \mathbf{f}_i | = (\epsilon_0^{-1}) \sum_i | \vec{\mathbf{p}}_i | \cdot \partial \mathbf{f}_i / \partial E$

$$= \epsilon_0^{-1} \frac{ea}{2} \cdot \frac{d}{dE} \left( \frac{-\exp(-eaE/2k_B T) + \exp(eaE/2k_B T)}{\exp(eaE/2k_B T) + \exp(-eaE/2k_B T)} \right) = \epsilon_0^{-1} \frac{ea}{2} \frac{d}{dE} \tanh(eaE/2k_B T)$$

$$= \epsilon_0^{-1} \frac{(ea)^2}{4k_B T} \text{sech}^2(eaE/2k_B T)$$

**(2) Elasticity**

(a)  $e_{yy}$  and  $e_{zz}$  are identically zero from the definition of “clamped”

(b) To derive the stress terms, we first write the form of the stiffness matrix from the clues given for a

$$\text{cubic solid: } \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

By inspection, we see that  $P_{xx} = C_{11}e_{xx} + C_{12}e_{yy} + C_{12} + e_{zz} = C_{11}e_{xx}$

$$P_{zz} = C_{12}e_{xx} + C_{12}e_{yy} + C_{11}e_{zz} = C_{12}e_{xx}$$

(c) Assuming  $e_{xx} = 1 \times 10^{-2}$ ,  $C_{11} = 1.66 \times 10^{11}$  N/m<sup>2</sup>,  $C_{12} = 0.64 \times 10^{11}$  N/m<sup>2</sup> we get

$$P_{xx} = 1.6 \times 10^9 \text{ N/m}^2, \quad P_{zz} = 0.64 \times 10^9 \text{ N/m}^2$$

Fundamental constants:

$$k_B = 1.38 \times 10^{-23} \text{ J/K}; \quad h = 6.626 \times 10^{-34} \text{ J-s}; \quad e = 1.602 \times 10^{-19} \text{ C}; \quad m_e = 9.11 \times 10^{-31} \text{ KG}; \quad \epsilon_0 = 8.85 \times 10^{-12} \text{ F/m.}$$

- (d) If replaced by an isotropic homogeneous solid, we still have 12 nonzero stiffness matrix elements. But there now only two independent ones.
- (e) if clamps are removed,  $P_{xx} = Y e_{xx}$  where  $Y$  is Young's modulus.  $e_{zz} = e_{yy} = \sigma e_{xx} = \sigma P_{xx}/Y$ .

### (3) Lattice Waves

- (a) **Two types** of elastic waves can propagate: (1) **compressional**, and (2) **shear**. With compressional, the polarization is longitudinal (deformation along propagation direction). With shear, the polarization is transverse (deformation perpendicular to propagation direction).
- (b) The **compressional** always has the higher velocity, and is so much higher than the analogous (sound) waves in fluids because solids have so much higher *stiffness* than fluids.
- (c) By atomic theory, there are **four** total wave types: (1) **longitudinal acoustic** (corresponding to compressional elastic), (2) **transverse acoustic** (corresponding to shear elastic), (3) **longitudinal optical**, and (4) **transverse optical**. By atomic theory, there are **three acoustical lattice waves**. And there are **3p-3 optical lattice waves**, where  $p$  is the number of atoms per primitive unit cell. For the given solid with  $p = 5$ , we get **twelve** optical waves and **fifteen** total (lattice) waves. We expect **one** longitudinal wave per atom per primitive cell. So of the **fifteen** total, **five are polarized longitudinal and ten are polarized transverse**.
- (d) By equipartition, there is a contribution of  $(1/2)k_B T$  per "degree-of-freedom". Each longitudinal wave provides two such degrees-of-freedom, one for kinetic energy and one for potential. **So each longitudinal wave provides  $k_B T$  of energy. Each transverse wave has the same contribution,  $k_B T$ .** So by simple multiplication, **we get  $15k_B T$  of energy for all the waves**, and  **$15N_C k_B T$  energy for the entire solid** where  $N_C$  is the number of primitive unit cells in the solid. {Another acceptable way to work the problem is by considering the atoms as energy bearers. Each atom provides 6 degrees of freedom (3 from potential energy, 3 from kinetic). So each atom provides  $3k_B T$  of total energy. So for 5 atoms per primitive cell, we get  $15k_B T$  per primitive cell, or  $15N_C k_B T$  total energy}. The resulting heat capacity of the solid from all lattice waves is just  **$C_V \approx dU/dT = 15N_C k_B$** .
- (e) Silicon has the diamond structure and GaAs the zincblende. So both have one longitudinal acoustic wave, two transverse acoustic, one longitudinal optic, and two transverse optics (six total waves). Aluminum is fcc, so only has one longitudinal acoustic and two transverse acoustic (three total). GaAs should have the strongest interaction with IR radiation because its optical lattice waves are polar in nature, Ga and As being partially ionic, so interact strongly with electromagnetic fields.

### (4) Sommerfeld-Fermi Model.

- (a) To get the density of states, we note: #states/length in  $k$  space =  $L/2\pi$ . So,  $N(k) = \left(\frac{L}{2\pi}\right) 2k$

(factor of 2 for positive and negative  $k$ ). Since  $U = \frac{\hbar^2 k^2}{2m}$ ,  $N(U) = \frac{L}{\pi} \frac{(2mU)^{1/2}}{\hbar}$ , and

$$D_{1d}(U) = \frac{dN}{dU} = \frac{m^{1/2} L}{2^{1/2} \pi \hbar} U^{-1/2} \text{ which diverges as } U \rightarrow 0. \text{ But this is an integrable singularity so it}$$

should not cause problems in statistical averages, which are always integrals (or summations)

- (b) In one dimension, the total number of electrons as a function of Fermi Energy is

$$N_{1d} = \int_0^\infty 2 \cdot f_{FD}(U) D(U) dU \approx \int_0^\infty 2 \cdot D(U) U \cdot \theta(U) \theta(U_F - U) dU = \int_0^{U_{F,0}} 2D(U) dU$$

$$\text{So by substitution of } D_{1D} \text{ from (a) } N_{1D} = \sqrt{2m^*} \cdot \frac{L}{\pi \hbar} \int_0^{U_{F,0}} U^{-1/2} dU = \sqrt{2m^*} \cdot \frac{2L(U_{F,0})^{1/2}}{\pi \hbar}$$

$$\text{So the line density is } \rho_{1D} \equiv \frac{N_{1d}}{L} = \sqrt{2m^*} \cdot \frac{2(U_{F,0})^{1/2}}{\pi \hbar}$$

- (c) If  $\rho_{1D} = 1 \times 10^6 \text{ cm}^{-1}$  ( $1 \times 10^8 \text{ m}^{-1}$ ), then  $U_{F,0} = 2.25 \times 10^{-21} \text{ J} = 0.014 \text{ eV}$ . The Fermi velocity is  $v_F =$

#### Fundamental constants:

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$$(2U_{F0}/m^*)^{1/2} = 2.7 \times 10^5 \text{ m/s.}$$

(d) The mean kinetic energy is given by:

$$\langle U \rangle \approx \int_0^\infty 2 \cdot D(U) U \theta(U) \theta(U_F - U) dU = \int_0^{U_{F0}} \sqrt{\frac{m^*}{2}} \frac{2L}{\pi \hbar} U^{1/2} dU = \frac{\sqrt{2m^*}}{3} \frac{2L}{\pi \hbar} U_{F0}^{3/2}. \text{ But from}$$

$$\text{the result of (b), } \sqrt{2m^*} \cdot \frac{2L}{\pi \hbar} = N_{1D} U_{F0}^{-1/2}, \text{ so that } \langle U \rangle = (1/3) N_{1D} U_{F0}.$$

(e) If  $U_{F0, \max}$  is 1.0 eV, we use (b) again to find a max line density:  $\rho_{1D, \max} = 8.4 \times 10^8 \text{ m}^{-1}$  or  $8.4 \times 10^6 \text{ cm}^{-1}$ .

### (5) Bloch Model

(a) For two electrons per unit cell, we would expect insulating behavior at low temperature since the  $n=1$  band would be just full, and there is gap separating it from the  $n=2$  band.

(b) For three electrons per unit cell, we would expect metallic behavior with the  $n=1$  band full and the  $n=2$  band half-full. The Fermi level would lie approximately midway up the  $n=2$  band.

(c) The group velocity can always be written  $v_g = \hbar^{-1} (dU/dk)$  in one dimension, or more generally,

$$\vec{v}_g = \hbar^{-1} (\vec{\nabla}_k U) \text{ in three dimensions?}$$

(d) The effective mass at any minimax point is defined by  $m^* = \hbar^2 (d^2U/dk^2)^{-1}$ . For the three bands shown, the effective mass of  $n=1$  is positive, and the effective masses of  $n=2$  and  $n=3$  are negative. Because it clearly has the smallest curvature (i.e., second derivative), the  $n=3$  band has the largest magnitude of effective mass at  $k=0$ .

(e) The Bloch wavefunction is  $\Psi_{n,k}(\vec{r}) = \phi_{n,k}(\vec{r}) e^{i\vec{k} \cdot \vec{r}}$  where  $\vec{k}$  is the crystal wavevector,  $\phi_{n,k}$  is the cell-periodic (or atomic) function, and  $n$  is the band index. The translation property is  $\Psi(\vec{r} + \vec{R}) = e^{i\vec{k} \cdot \vec{R}} \Psi(\vec{r})$  where  $\vec{R}$  is any primitive lattice vector.

### (6) Semiconductor Band Statistics

(a) GaN has a spherical conduction band so the electronic density-of-states is given by  $D(U)$ , so with spin degeneracy included the density of states is  $2 \cdot V(m^*)^{3/2} U^{1/2} / [(2)^{1/2} \pi^2 \hbar^3]$  (no partial credit)

(b)  $m_d^*$  is the density-of-states mass, which is  $0.21 m_e$  for GaN since the conduction band is assumed spherical.  $M$  is the equivalent number of electron "valleys" (or "pockets"), which is 1 for GaN. Evaluating the expression, we get  $N_C(300 \text{ K}) = 2.4 \times 10^{24} \text{ m}^{-3} = 2.4 \times 10^{18} \text{ cm}^{-3}$ .

(c) The hydrogenic model results in a proton and electron embedded in the otherwise perfect crystal lattice of the host. Hence, we can use the (vacuum) hydrogen energy levels by making the substitution  $m_e \rightarrow m^*$  and  $\epsilon \rightarrow \epsilon_r \epsilon_0$ , so that  $\phi_B = -m^* e^4 / [8(h\epsilon_r \epsilon_0)^2] = -3.07 \times 10^{-21} \text{ J} = -0.019 \text{ eV}$

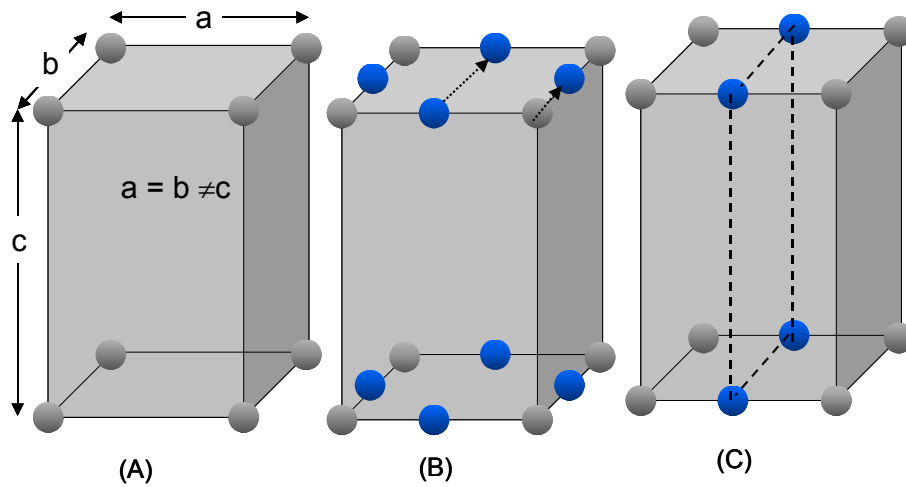
(d) When the Fermi level lies at the donor energy,  $U_F - U_C = \phi_B$ , so that  $n = N_C \exp(-\phi_B/k_B T) = 1.15 \times 10^{24} \text{ m}^{-3} = 1.15 \times 10^{18} \text{ cm}^{-3}$ .

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**(7) Bonus Problem: Crystals**

- (a) Yes, the elongated crystal structure is a *tetragonal* Bravais lattice, the coordination number is two if  $c < a$ , and is four if  $c > a$ . The primitive unit cell has volume  $abc = a^2c$ .
- (b) With the additional edge atoms, we no longer have a Bravais lattice. To prove this, consider the configuration seen from the two atoms along the vectors shown in the (B) below. Clearly, the configuration seen from one atom is not the same as the configuration seen from the other atom.
- (c) By eliminating the four atoms along opposite edges as shown in (C), the crystal structure becomes a Bravais lattice once again, this time an *orthorhombic* lattice having a coordination number of two (no matter what the  $c/a$  ratio), and a primitive unit cell volume  $(a/2)bc = a^2c/2$ .
- (d) But if the blue atoms in (C) are not the same as the gray atoms, we no longer have a Bravais lattice since space does not look the same looking from a gray atom towards a blue atom as it does from a blue atom towards a gray atom.



*This figure or something similar should be included if the student is to receive full credit.*

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