Key for Final Examination for

Introduction to Nano Science and Technology A(1)

January 11, 2010

1. (a) Write down the distribution functions of Boltzmann, Bose, and Fermi, respectively, and compare them with their most important attributes. (10 points)

   (b) Describe the physical meaning of the Fermi energy (E_F) for a Fermi system. (3 points)

   (c) For a metal at T = 0 K, show that, using the free electron gas model, the average energy of an electron is $3E_F/5$. (7 points)

Ans:

(a)

	Boltzmann	Bose	Fermi
Distribution Function	$e^{-E/kT}$	$\dfrac{1}{e^{\alpha}e^{E/kT}-1}$	$\dfrac{1}{e^{(E-E_F)/kT}+1}$
Basic characteristics	Applied to distinguishable particles	Applied to indistinguishable particles not obeying exclusion principle	Applied to indistinguishable particles obeying exclusion principle.
Examples	gas systems	photon gas	electron gas

(b) Based on the Fermi distribution function, the Fermi energy is defined as the energy at which the occupied states are separated with the unoccupied states at T=0.

(c) The total energy for the free electron gas containing N electrons is:

$$\bar{E} = \int_0^{\epsilon_F} \epsilon \frac{dN}{d\epsilon}\, d\epsilon \quad , \quad \epsilon_F \text{ is determined by } N.$$

$$= \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^{\epsilon_F} \epsilon^{3/2}\, d\epsilon$$

$$= \frac{2}{5}\frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon_F^{5/2}$$

$$\epsilon_F = \frac{\hbar^2}{2m}\left(3\pi^2 \frac{N}{V}\right)^{2/3}$$

$$\Rightarrow N = \frac{V}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon_F^{3/2}$$

The average energy of an electron

$$E/N = \frac{3}{5}\epsilon_F$$ #

2. Consider the periodic two-dimensional solid with part of it as shown in the figure below. The white atoms form a square structure, and some black atoms sit on the hollow sites formed by four white ones.

(a) Draw the primitive unit cell and lattice vectors in two different ways. (5 points)

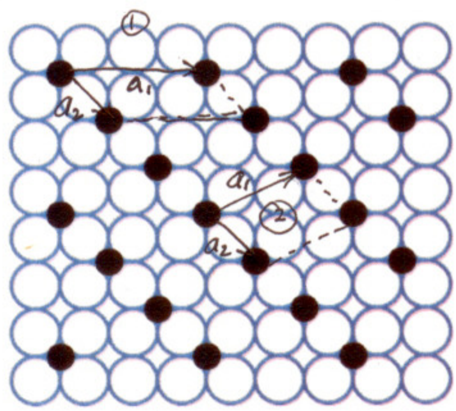
(b) Let the diameter of the white atoms be d. What is the size (area) of a primitive unit cell in terms of d? (5 points)

(c) Draw the unit cell and lattice vectors (in terms of d) of the corresponding reciprocal lattice. (5 points)

(d) What is the size of a primitive unit cell in terms of d in the reciprocal lattice? (5 points)

Ans:

(a)

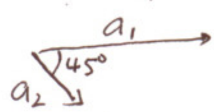


(b) $|\vec{a}_1| = 3d$

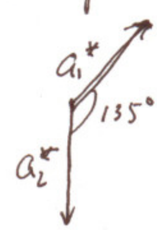
$|\vec{a}_2| = \sqrt{2}\, d$

$A = |\vec{a}_1 \times \vec{a}_2| = \underline{3d^2}$.

(c) Real Space



Reciprocal Space



$\vec{a}_1^* \cdot \vec{a}_1 = 2\pi$

$\Rightarrow |\vec{a}_1^*||\vec{a}_1| \cos 45° = 2\pi$

$\Rightarrow |\vec{a}_1^*| = \underline{2\pi \cdot \sqrt{2}/3d}$.

Likewise, $|\vec{a}_2^*||\vec{a}_2| \cos 45° = 2\pi$

$\Rightarrow |\vec{a}_2^*| = 2\pi \cdot \sqrt{2}/\sqrt{2}d = \underline{\frac{2\pi}{d}}$.

(d) $A^* = |\vec{a}_1^* \times \vec{a}_2^*|$

$= |\vec{a}_1^*|\,|\vec{a}_2^*| \sin 135°$

$= \frac{2\sqrt{2}\pi}{3d} \times \frac{2\pi}{d} \times \frac{\sqrt{2}}{2} = \underline{\frac{4\pi^2}{3d^2}}$

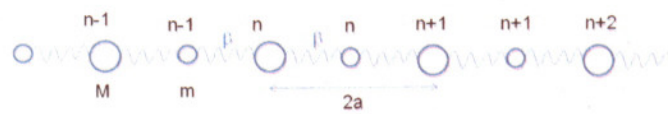
3. In a diatomic linear chain (as sketched below), the solution for the equation of longitudinal motion is

$$\omega^2 = \beta\left(\frac{1}{m}+\frac{1}{M}\right) \pm \beta\sqrt{\left(\frac{1}{m}+\frac{1}{M}\right)^2 - \frac{4\sin^2 ka}{Mm}}.$$

(a) Sketch the dispersion curve of this chain moving in one dimension in the first Brillouin zone. (5 points)

(b) Indicate the intersection points at $k = 0$ and the zone boundary, and describe the atomic motions corresponding to these points. (10 points)

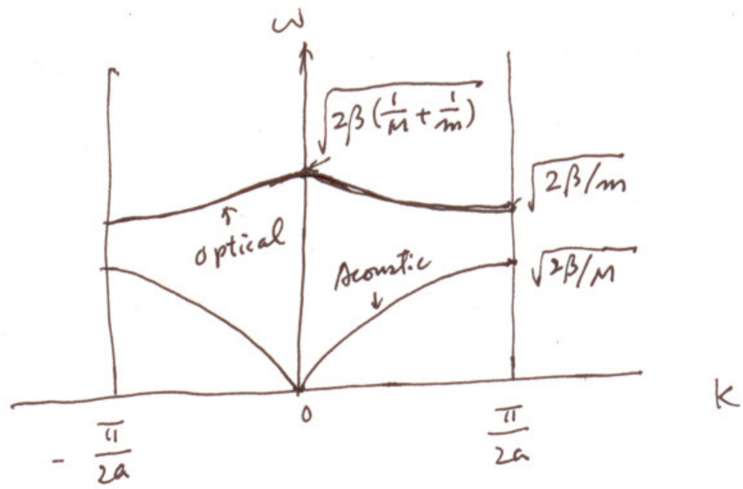
(c) For a sheet of graphene, if the carbon atoms are allowed only in-plane motion, how many branches are there for acoustic and optical vibrations, respectively? (5 points)



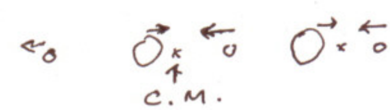
Ans:

(a)

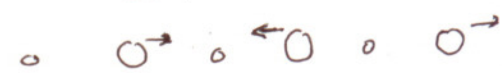
(b)



(c) For $\omega = \sqrt{2\beta\left(\frac{1}{M}+\frac{1}{m}\right)}$,



For $\omega = \sqrt{2\beta/M}$



For $\omega = \sqrt{2\beta/m}$

(c) For Graphene, ~~unit~~ lattice contains two carbon atoms. Since these atoms are allowed to move in the plane, the total freedoms of motion for atoms in a unit cell will be 4; two branches for the acoustic vibration and two branches for the optical.

4. (a) Use the "nearly free electron gas model" to describe the origin of the energy gap in the band theory. (10 points)
   (b) Why are metallic solids mostly opaque, covalent solids sometimes opaque, and ionic solids hardly ever opaque to visible light? (5 points)
   (c) When a photon is absorbed by a semiconductor, an electron-hole pair will be created and both of them can contribute to the conductivity of the sample. Compare the hole to the electron of this pair, what will be their relations in terms of wavevector, velocity, mass, and charge? (5 points)

Ans:

(a) In the nearly free electron gas model, a small periodic potential is introduced. $U(\vec{r}+\vec{T}) = U(\vec{r})$
This periodic potential will cause the electrons having wavectors close to the values of Brillouin boundaries to experience strong reflection. Right at the Brillouin Zone boundary, two standing wavestates can co-exist, and each corresponding to different distributions of electron density. Subsequently, they represent two different states with different energy at the zone boundary. So, energy gap is created.

(b) metallic solids have no energy gap and will absorb visible light, so they appear opaque.
Covalent solids are usually semiconductors. Their energy gas can vary with temperature, so they appears opaque at higher temperature.
Ionic solids are insulators, which have wide bandgaps. They will not absorb any visible light and look transparent.

(c) $m_h = -m_e$; $v_h = v_e$; $K_h = -K_e$; $q_h = -q_e$.

5. Indium Phosphide (InP) has $E_g = 1.4$ eV; dielectric constant $\varepsilon = 10$; electron and hole effective masses $m_e^* = m_h^* = 0.07m_e$. Calculate:
   (a) The exicton binding energy. (7 pts)
   (b) The distance of the electron-hole pair in term of Bohr radius (a_0). (5 pts)
   (c) Imagine an optical absorption experiment has been performed on this system. Sketch a diagram with absorption coefficients vs. photon energy to indicate the exciton state and the energy gap. (5 pts)
   (d) Discuss briefly about the optical properties of an InP quantum dot with reference to its bulk counterpart. (3 points)

Ans:

(a) $$E_c - E_e = 13.6 \times \left(\frac{\epsilon_0}{\epsilon}\right)^2 \times \left(\frac{\mu^*}{m_e}\right) \text{ (eV)}$$

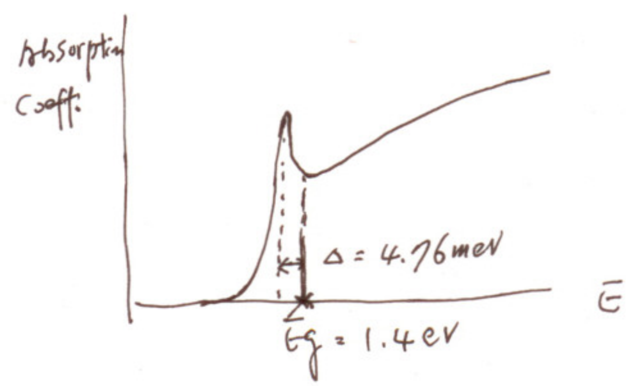
$$\frac{1}{\mu^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*} = \frac{2}{0.07 m_e} \Rightarrow \mu^* = 0.035\, m_e$$

$$\Rightarrow E_c - E_e = 13.6 \times \frac{1}{100} \times 0.035 = \underline{4.76 \text{ (meV)}}$$

(b) $$a_e = a_0 \times \left(\frac{m_e}{\mu^*}\right) \times \left(\frac{\epsilon}{\epsilon_0}\right) \text{ (Å)}$$

$$= 0.53 \times \frac{1}{0.035} \times 10 = \underline{151 \text{ Å}}$$

(c)



(d) The optical spectrum of an InP quantum dot, comparing to its bulk material, can have both blue-shift and red-shift features:

i) Blue-shift: due to the size effect on widening the bandgap; or the confinement effect on the formation of exciton.

ii) Red-shift: due to the surface effect; surface atoms have less coordinate number of atoms and dominate the vibration spectrum.