**Your name: _____ Your Score: _____**

1. **Structure and mechanics of crystalline solids (20 points)**
a.(8pts) The following is the unit cell of GaAs (zincblende structure). On average how many Ga atoms are there and how many As atoms are there per unit cell? What is the coordination number? The following also shows the atomic arrangement on a (100) plane on the surface of the shown unit cell. Please draw a similar image of atomic arrangement on a (111) plane of this unit cell, and label which atoms are Ga and which are As, and label the side lengths of this (111) plane.
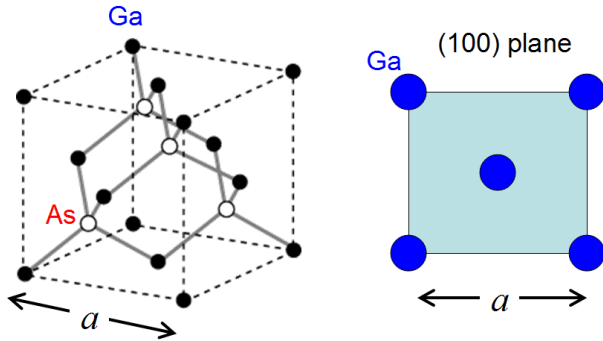
The number of Ga = the number of As = 4 (2pts)
The coordination number = 4 (2pts)
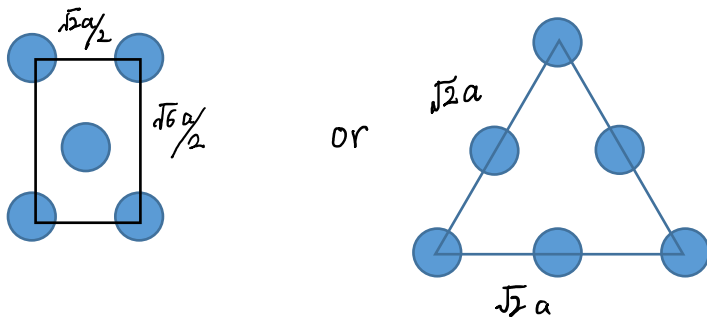
Draw (111) plane (2pts)
Label the side length of unit cell (2pts)

b.(12pts) Explain with text and schematics the bonding in (1) diamond, (2) NaCl, and (3) Cu.

(1) diamond
Covalent bonding + schematics (2pts)
Need to mention that electrons are shared between atoms (2pts)
Suggest schematics:

(2)NaCl
Ionic bonding + schematics (2pts)
Need to mention that electrons are transferred between atoms (2pts)
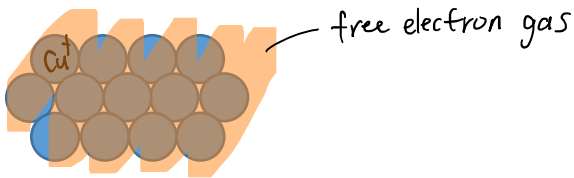Suggested schematics:


(3)Cu
Metallic bonding + schematics (2pts)
Need to mention that electrons has a motion similar to free gas (free electron gas) (2pts)
Suggested schematics:

2. Electrical transport (20 points)
a.(10pts) Explain in a few lines the principle of Hall effect. A schematic is shown below. Add more schematics to help your explanation if necessary. What physical quantities are this used to measure?
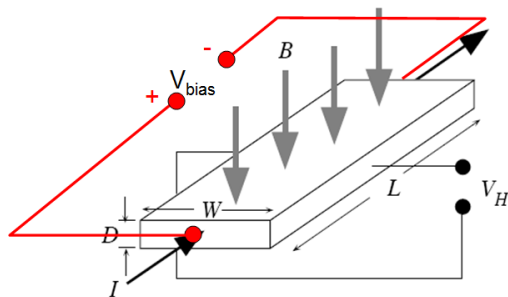
Hall effect: the production of a **voltage difference (2pts)** (or electric field or Hall voltage) across an electrical conductor, transverse to an **electric current (1pts)** (or motion of the charge carriers) in the conductor and to an **applied magnetic field (2pts)** perpendicular to the current.

Physics quantities that Hall effect can measure:
Mobility (must include, 3pts) + one other (2pts) (electrical conductivity, charge carrier density, n/p type, measure magnetic field)

Some answers are: effective mass, mean free time; Ok, technically yes (optical hall effect) but in a different setup.

b. (10pts) If we have both free electrons (negatively charged) and free holes (positively charged) inside a material, under a given voltage bias (V_{bias} as shown above), will the electron and hole tend to add or cancel each other's contribution to the material electrical conductivity? Will their contributions to Hall effect (i.e., the Hall voltage V_H) tend to add or cancel? Explain in details (Hint, draw a schematic of forces may help).

(1) electrical contribution:
Add (2pts); should argue from the perspective that that electron (negatively charged) and hole (positively charged) in current are driven **in opposite direction (3pts)** along x-axis

Common mistakes for argument:
a. give equation as: $\sigma = n_e e \mu_e + n_h e \mu_h$ ←this is just another way to say that electron and hole will add their contributions to electrical conductivity (restating the phenomenon but not explaining the reason)
b. electrons + holes result in more charge carriers ←No, if electrons and holes move in the same direction within current. Even though the carrier density is high, the effective current will be less.

(2) Hall effect
Cancel (2pts); should argue from the perspective that electrons and holes will accumulate at **the same side (3pts)** of conductor driven by Lorenz force.

Common mistakes: do not consider the charge polarity when determining the direction of Lorenz force

3. Thermal transport (20 points)

a. (5pts) The thermal conductivity of a crystalline material has two components, contribution from lattice, $k_{lattice}$, and contribution from electrons $k_{electronic}$. Explain in a few lines the physical mechanism of the fact that $k_{electronic}$ is proportional to the electrical conductivity σ of the material times temperature T (i.e., the Weideman-Franz Law).

(1) 3pts: $k_{electronic}$ is proportional to the electrical conductivity σ:
Need to explain from the perspective that electron carries both charge (σ is related the charge transportation) and energy (k is related to energy transportation)

Cases:
Mention: **electron carries energy (+3pts)**
Mention: electron is the "shared" carrier but not explicitly pointing out that energy is the cargo that been carried (+1pts)

(2) $k_{electronic}$ is proportional to the temperature T:
Need to explain from the perspective that **the energy (thermal energy or kinetic energy) that electron carries is proportional to k_BT (2pts)** (or increase with temperature)

Common mistakes: when temperature rises, electron moves faster (has larger velocity)
The fact is correct, but this won't help to explain why:

$$\frac{\kappa}{\sigma} \propto T$$

If velocity increases, then $k_{electronic}$ and σ will increases to the same extent. This is because $k_{electronic}$ is proportional to σ but won't help explain the dependency on T of $k_{electronic}$
Also, if you do real calculations, velocity term would eventually be cancelled out. Only energy term remains in the final expression.

Another mistake is to say charge carrier density increase with T. Not always true and not in a relation as proportional to T. In extrinsic undegenerate semiconductor, this is true. But in metal, all valence electrons have already been freed/excited by forming metallic bondings. Thermal energy won't be high enough to excite core electrons therefore the number of electrons won't change in metal (or degenerate semiconductor).

b. (15pts) $k_{lattice}$ is low at low temperatures, and low at high temperatures, while peaks at some intermediate temperature (tens of K). Explain in details what physics causes the low $k_{lattice}$ at very low temperatures, and what process causes the low $k_{lattice}$ at very high temperatures. (Hint, remember the phonon scattering process, and $k_{lattice} = C_v \cdot v \cdot l / 3$ $k_{lattice} = C_v \cdot v \cdot l / 3$, where C_v = specific heat, v = sound velocity, and l = phonon mean free path).

2pts (1) show diagram of Cv vs T (2pts) [OR mention **at low T Cv is proportional to T³ (increasing) (1pt)** and **at high T Cv = 3kВn (or constant)(1pt)**]
2pts (2) show diagram of l vs T (2pts) [OR mention **at low T l is limited by boundary scattering therefore constant (1pt)** and **at high T l is inversely proportional to T (or decreasing)(1pt)**]
3pts (3) show diagram of v vs T (3pts) or mention that velocity of phonon is constant over all T
Hence, with three diagrams you can argue that:
4pts (4) low $k_{lattice}$ at very low temperatures is due to low Cv at low T (2pts). The physics is: at low T, phonon mode can not be fully excited (or density of phonons is low at low T) (2pts)
4pts (5) low $k_{lattice}$ at very high temperatures is due to low l at high T (or phonon-phonon scattering or Umklapp scattering) (2pts). The physics is: at high T, the density of phonon is high due to enhanced thermal excitation (l is inversely proportional to phonon density) (2pts).
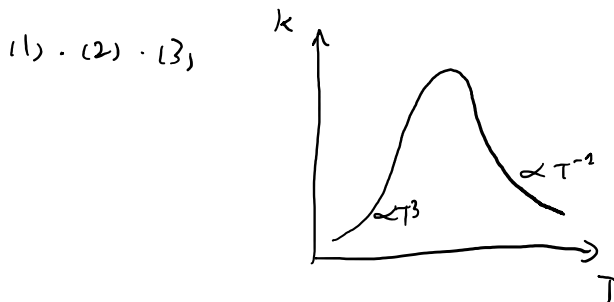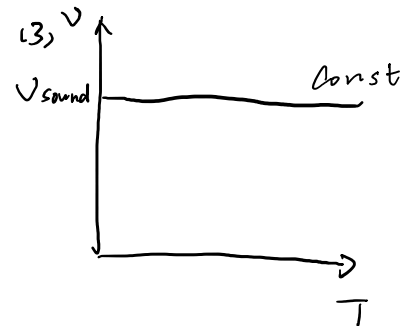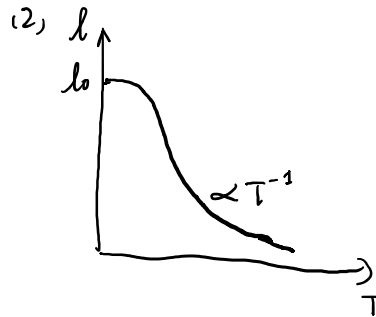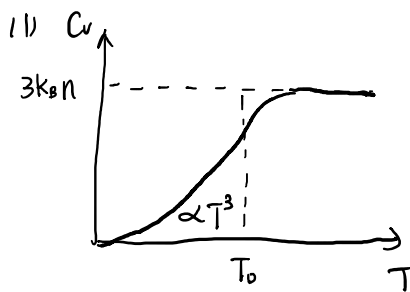
4. Quantum physics (40 points)

a. (10pts) Using Heisenberg's uncertainty principle, estimate (i.e., find an approximate expression without using the Schordinger equation solution) the value (in units eV) of ground state energy (E_1) of an electron confined in an infinitely-deep 1D square well with well width $L = 1$ nm. (Hint, we know that you don't remember the value of Planck's constant (h) and of electron mass (m_e); but it's helpful to remember that $\hbar \cdot c = 1973 \; eV \cdot Å$: you can remember that by the fun fact that the year 1973 is the year when the first mobile phone call was made in Motorola; and $m_e c^2 = 0.51$ Mega-eV $= 0.51 \times 10^6 eV$ is electron's rest energy: that's the immediate application of Einstein's E=mc^2. Then you can numerically estimate E_1. These two combined constants, plus a third one $e^2/\hbar c = 1/137$ called "fine structure constant", if you can remember, would be hugely useful for your future science/tech career, because you no longer need to remember the individual values of h, c, me, ε_0, e, etc).

$$\Delta p \cdot \Delta \ell \simeq \hbar \quad \overset{4pts}{} \quad , \quad \Delta \ell = L = 1 nm = 10 \, Å$$

$$\Rightarrow \quad \Delta p \approx \frac{\hbar}{L}$$

$$E_1 \simeq \Delta E = \frac{\Delta p^2}{2 m_e} \quad \overset{4pts}{} \quad = \frac{\hbar^2}{2 m_e L^2} = \frac{(\hbar c)^2}{2 (m_e c^2) \cdot L^2}$$

$$= \frac{(1973 \; eV \cdot Å)^2}{2 \times (0.51 \times 10^6 eV) \times (10 Å)^2} = 0.038 \; eV \quad \overset{2pts}{}$$
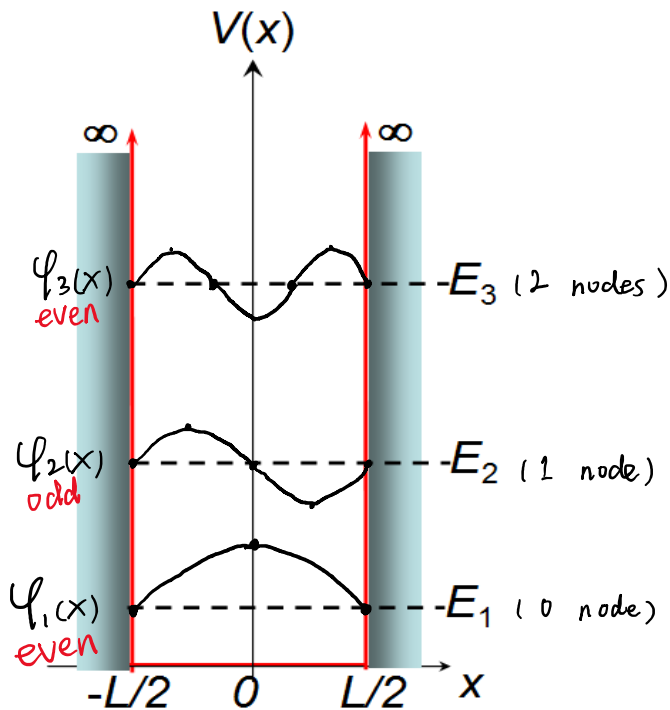
b. (5pts) At room temperature, will this electron mostly sit in the ground state, or have a significant probability to be thermally excited to higher energy levels (E_n with $n \geq 2$)? Show details. (Hint, Recall that E_n is proportional to n^2, hence $E_2 - E_1 = 3E_1$. Also remember that $k_B T = 0.026 eV$ at 300K.)

mostly sit in the ground (2pt)

$$E_2 - E_2 = 3E_1 = 3 \times 0.038 \; eV = 0.114 \; eV \; > \; 0.026 eV$$

3pt

c. (25pts) Draw schematically the wavefunction of the $\varphi_1(x)\,\varphi_1(x)$, $\varphi_2(x)\,\varphi_2(x)$ and $\varphi_3(x)\,\varphi_3(x)$ in the following plot. (Note that here $x=0$ is at the center, not the edge, of the well as exercised in class; please pay attention to the boundary condition and correct symmetry of each wavefunctions). If there is one electron sitting in the $\varphi_1(x)\,\varphi_1(x)$ state, we shine a beam of light with a broad range of wavelengths. The probability, $P(1 \to 2)\,P(1 \to 2)$, of promoting the electron to $\varphi_2(x)\,\varphi_2(x)$ state (called optical transition) is known to be proportional to $\langle 1|x|2 \rangle = \int_{-\infty}^{\infty} [\varphi_1(x)]^* \cdot x \cdot \varphi_2(x)dx \; \langle 1|x|2 \rangle = \int_{-\infty}^{\infty} [\varphi_1(x)]^* \cdot x \cdot \varphi_2(x)dx$. Show using the schematics of wavefunctions (rather than using equations), that $P(1 \to 2)\,P(1 \to 2)$ is nonzero while $P(1 \to 3)\,P(1 \to 3)$ must be zero. This is called the selection rule.

Selection rule :

1) $P(1 \to 2)$

$$\langle 1|x|2 \rangle = \int_{-\infty}^{\infty} \varphi_1^* \times \varphi_2(x)\, dx$$

$$= \int_{-L/2}^{L/2} \underset{even}{\varphi_1^*} \cdot \underset{odd}{x} \cdot \underset{odd}{\varphi_2(x)}\, dx$$

$$= \int_{-L/2}^{L/2} [\,even\,]\, dx \;\neq 0$$

2) $P(1 \to 3)$

$$\langle 1|x|3 \rangle = \int_{-\infty}^{+\infty} \varphi_1^* \cdot x \cdot \varphi_3(x)\, dx$$

$$= \int_{-L/2}^{L/2} \underset{even}{\varphi_1^*} \cdot \underset{odd}{x} \cdot \underset{even}{\varphi_3(x)}\, dx$$

$$= \int_{-L/2}^{L/2} [\,odd\,]\, dx = 0$$

10pts: draw schematically the wavefunction of the $\varphi_1(x)$, $\varphi_2(x)$ and $\varphi_3(x)$

15pts: argue selection from the perspective of parity of functions under the integral

(The last question: "Show using the schematics of wavefunctions" can have two ways to interpret: 1) draw schematics to show selection rule; or 2) use the schematics of wavefuntion from (1) to show selection rule. Therefore, we decide it is not necessary to show schematics)

Schematics :

P(1→2) :

P(1-3) :