This is a closed book exam. You are allowed to use both sides of a single 8.5"x10" sheet of paper for formula and constants. Calculators are only allowed for numerical computation only and not for storage of formulae. Clearly state all approximations and assumptions. You will only be graded for work shown. **Good Luck!**
Problem 1 (20 pts. total)
Consider a 1.0mm$^3$ cube of KCl crystal with an average atomic density of 1.949x10$^{19}$/mm$^3$. Assume the bulk elastic modulus is 1.88x10$^{10}$ Nm$^{-2}$ and the energy vs. atomic separation is approximated by the following repulsion and attraction terms:

\[
\text{Repulsion: } \frac{A}{r^9}, \quad \text{Attraction: } \frac{B}{r} \\
\text{with } B = \frac{1.75q^2}{4\pi\varepsilon_0}
\]

Part A (10 pts.) Calculate the separation of the K$^+$ and Cl$^-$ atoms

\[
c = -\frac{1}{9r_0} \left( \frac{\partial^2 E}{\partial r^2} \right)_{r=r_0} \\
= -\frac{1}{9r_0} \left( \frac{\partial^2 \left( \frac{A}{r^9} - \frac{B}{r} \right)}{\partial r^2} \right)_{r=r_0} \\
= -\frac{9}{9r_0^3} \frac{B}{r_0} \left( \frac{1}{9} - 1 \right)
\]

\[
r_0 = \sqrt[4]{\frac{B}{c} \left( \frac{1}{9} - 1 \right)}, \quad \text{where } c = 1.88 \times 10^{10} \text{ Nm}^{-2} \text{ and } B = \frac{1.75q^2}{4\pi\varepsilon_0} = 2.567 \times 10^{-38}
\]

\[
r_0 = \sqrt[4]{\frac{2.567 \times 10^{-38}}{1.88 \times 10^{10}} \left( \frac{1}{9} - 1 \right)}
\]

\[
r_0 = 3.717 \times 10^{-10} \text{ m}
\]
Part B (10 pts.) Calculate the cohesive energy (the minimum of the energy vs. atomic separation) of a K⁺-CL⁻ bond

\[ E_c = \frac{B}{r_0} \left( \frac{1}{9} - 1 \right) \]

\[ = \frac{4.037 \times 10^{-28}}{3.717 \times 10^{-10}} \left( \frac{1}{9} - 1 \right) \]

\[ = -9.655 \times 10^{-19} \text{J} \]

\[ = -6.026 \text{eV} \]

Part B (10 pts.) How much would the Fermi Level from part A change if the temperature of the metal were changed to room temperature (about 300K)?

The Fermi level would not change appreciably from zero degrees to 300K. As we saw later in the course, it takes much higher temperatures to change the Fermi Level appreciably.

Part C (10 pts.) In order to achieve a thermionic emission current of 1kA/cm² what would the temperature of the metal bar have to be raised to?

\[ J = 1 \times 10^{3} \text{A/m}^2 = A_{0}(1 - e^{-k_{B}T/2}) \cdot \frac{k_{B}}{h} \cdot k_{B} \]

\[ T = \left( \frac{2}{A_{0}(1 - e^{-k_{B}T/2}) \cdot \frac{k_{B}}{h}} \right)^{1/3} \]

\[ T = \left( \frac{2}{1.2 \times 10^{-8} \cdot (0.9)} \right)^{1/3} \]

\[ T = 9.26 \text{K} \]

The curve has a zero at \( T = 1823.73 \text{K} \).
Problem 2 (40 pts.)
Consider a metal bar that has a free electron density of $10^{22}$ cm$^{-3}$ and a work function equal to 2eV.

Part A (10 pts.) Calculate the Fermi Level at temperatures near absolute zero

$$E_F = \frac{\hbar^2}{2m} \left( \frac{3}{8\pi} N \right)^{\frac{2}{3}}$$

$$= \frac{(6.626 \times 10^{-34})^2}{2 \cdot (9.11 \times 10^{-31})} \left( \frac{3 \times 10^{22}}{8\pi \text{ cm}^3 \text{ m}^-3} \right)^{\frac{2}{3}}$$

$$= 2.41 \times 10^{-37} \cdot 5.177 \times 10^{18}$$

$$= 2.71 \times 10^{-19}$$

$$= 1.69eV$$

Part B (10 pts.) How much would the Fermi Level from part A change if the temperature of the metal were changed to room temperature (about 300K)?

The Fermi level would not change appreciably from zero degrees to 300K. As we saw later in the course it takes much higher temperatures to change the Fermi Level appreciably.

Part C (10 pts.) In order to achieve a thermionic emission current of 1kA/cm$^2$ what would the temperature of the metal bar have to be raised to?

$$J = 1 \times 10^7 A/m^2 = A_0(1 - r)T^2e^{-\frac{E_F - \varphi}{k_BT}}$$

$$T^2e^{-\frac{E_F - \varphi}{k_BT}} = \left( \frac{1 \times 10^7}{A_0(1 - r)e^{\varphi/k_BT}} \right)$$

$$= \frac{4\pi \alpha m_k \varphi}{h^3} = 1.2 \times 10^6 A \cdot m^2 \cdot K^{-2}$$

$$T^2e^{-\frac{3.204 \times 10^{19}}{1.38 \times 10^{-23}/T}} = \left( \frac{1 \times 10^7}{1.2 \times 10^6 \cdot (0.9)} \right)$$

$$T^2e^{-\frac{23.217.39}{T}} = 9.26$$

$$T^2e^{-\frac{23.217.39}{T}} - 9.26 = 0$$

has a zero at $T = 1823.73$ K
Part D (10 pts.) Calculate the applied electric field required to increase the emission current density to 2kA/cm² at the temperature found in Part C.

Applying a field \( E \) at temperature \( T \) will change the emission current density to

\[
J = A_0 (1 - r) T^2 e^{-\frac{q \sqrt{\frac{qE}{A \pi e_0}}}{k_B T}}
\]

\[
= A_0 (1 - r) T^2 e^{-\frac{q \sqrt{\frac{qE}{A \pi e_0}}}{k_B T}}
\]

\[
= 1 kA/cm^2 \times e^{-\frac{q \sqrt{\frac{qE}{A \pi e_0}}}{k_B T}}
\]

using the parameters and solution from previous part

\[
2 = e^{-\frac{q \sqrt{\frac{qE}{A \pi e_0}}}{k_B T}}
\]

\[
E = \left( \frac{k_B T}{q} \ln 2 \right)^2 \frac{4 \pi e_0}{q}
\]

\[
= \left( \frac{1.38 \times 10^{-23} (23,217.39)}{1.6022 \times 10^{-19}} \ln 2 \right)^2 \frac{4 \pi 8.85 \times 10^{-12}}{1.6022 \times 10^{-19}}
\]

\[
= 8.23 \times 10^{-6} V/m
\]
Problem 3 (40 pts.)
Consider the band theory models we discussed in class (Kronig-Penny, Ziman and Feynman). Each band theory model comes to the same conclusion (existence and structure of energy bands) using different mathematical language and physical pictures. The following questions are related to these models.

Part A (10 pts.) Describe in one brief paragraph for each model, the basis (e.g. mathematical description, physical description, etc.) and the assumptions made. Draw a simple picture with each paragraph to illustrate the basis for each model.

1. Kronig-Penny
   Fig 7.5
   Periodic potential
   Electron wavefunction
   \( \psi_k(x) = e^{ikx} \psi(x) \)
   Solution
   Allowed bands
   Forbidden bands

2. Ziman
   Fig 7.8
   Electron wavefunction
   \( \psi_k(x) = e^{ikx} \) (plane wave)
   \( 2a \sin \theta = n \lambda \) (Bragg reflection)
   This model predicts the width of the bandgaps.

3. Feynman
   Fig 7.11
   Energy level splitting from coupling of adjacent atoms.
   This model predicts the width of the allowed energy bands, and it also gives E-k diagram for negative k.
Part B (10 pts.) Draw the resulting $E$ vs. $k$ plot for each of the three models indicating all key values on the axis and the energy values on the curves themselves using the mathematical symbols used for each model. Make sure to label your plot with the model, the axis labels and indicate the key values on both the $E$- and $k$-axis.

Kronig-Penney

Ziman

Feynman

Part C (10 pts.) Only one model was useful for predicting the existence of energy band structures for many atoms, which one? This model assumed coupling (for the one-dimensional case) of only nearest neighbor atoms, write down the basic differential equation that describes how these atoms are coupled.

\[ i\hbar \frac{d\psi_j}{dt} = E_j\psi_j - A\psi_{j-1} - A\psi_{j+1} \]
Part D (10 pts.) The $E$ vs. $k$ plot for the lowest energy band (starting at $E_1$) for the model from part C is drawn for $+k$ and $-k$ values. Draw this picture indicating all key values and aspects for the lowest energy band and next band up (using $E_2$). Describe how this picture is related to the $E$ vs. $k$ plots for the other two models (be as specific as you can). The curvature of this $E$ vs. $k$ curve is related to what key concept that we learned about in class?

Curvature of the $E$-$k$ plot gives effective mass.