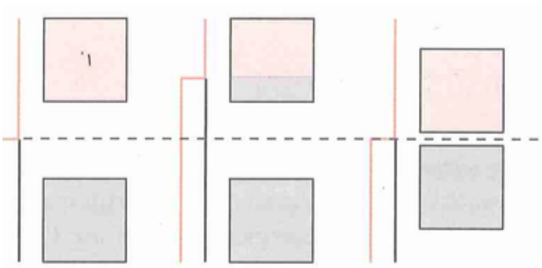
Electrical properties of solids - QM approach

1. The energy band model often refers to the *conduction band* and the *valence band*. The valence band is the highest energy band that would be completely full at zero temperature. The conduction band is the band just above the valence band.

   For each of the following energy band schematics
   (a) label the valence and conduction bands
   (b) identify the material as either a conductor, insulator or semiconductor.

2. The outermost shell of a material has the following configuration: $2s^1$. There's exactly 1 mol of this material in a solid piece.

   In the 2s band, how many
   (a) energy states are there?
   (b) electron states are there?

   (c) How full is the 2s band?

3. The 3s energy band in sodium has a width of 6.44eV. A sample of sodium has 2.65×10^{22} atoms in it. Calculate the spacing between adjacent energy levels.

   (2.4×10^{-22} eV)

4. Explore the behavior of the Fermi-Dirac distribution on desmos. To make things simpler, plot the following:

$$f(x) = \frac{1}{e^{(x-x_f)/T} + 1}$$

   Add sliders for x_f and T, where $x, T \geq 0$.

   (a) Change x_f. What happens when you increase x_f? Sketch an example.
   (b) Change T. What happens when you increase T? Sketch an example.
   (c) For any $T > 0$, what's the probability that the state x_F is occupied?

5. Calculate the probability that the lowest energy state in the conduction band is occupied when $T = 300$K for
   (a) an insulator with an energy gap 5eV
   (b) a semiconductor with an energy gap of 1eV

   Here, it's easiest to use k_B in eV/K. Keep in mind that E_F is in the middle of the energy gap. That is, $(E_{\text{lowest conduction}} - E_F) = 2.5$eV for the insulator.

   ($10^{-42}, 10^{-8}$)

6. How does the energy band model

   (a) describe the difference between conductors and insulators?

   (b) explain why conductors conduct electricity well, while insulators don't?

7. Use words, a diagram and an equation to describe the (a) the Fermi energy, and (b)the Fermi-Dirac distribution.

8. It turns out that semiconductors have some electrons in occupying some states in the conduction band, and some empty states in its valence band for $T > 0$. Insulators, however, generally don't. Why?

---

9. The QM free electron model treats the electron as a particle in a box. That is, the particle is confined to the metal (the box), by infinitely high potential at the edges ($U \to \infty$ at the edge), and is in the presence of a constant potential $U = U_0$ when inside the metal.

   (a) When we talk about free electrons, which electrons are these? All the electrons in the metal? If not all, which ones?

   (b) What effect do the positive ions (that make up the lattice), have on the free electrons?

   (c) How does the free electron model treat electron-electron interactions?

10. The allowed energies in an infinite potential well ($U = 0$ inside the well, ∞ otherwise) are determined by the time independent Schrödinger equation (TISE). In 1D this is

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - U(x)\psi(x) &= E\psi(x) \\ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) &= E\psi(x) \end{aligned}$$

   (a) Show that $\psi(x) = A\sin(k_x x)$ is a solution to this 1D TISE.

   (b) Determine an expression for E.

   (c) Outside and at the edges of the well, $\psi(x \leq 0) = \psi(x \geq L) = 0$. Based on these boundary conditions, show that k_x can only take on certain values

$$k_x = \frac{n_x \pi}{L}$$

   where n_x is an integer.

11. The 2D infinite well [$U(x, y) = 0$ inside the well, ∞ otherwise] is described by

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x, y) = E\psi(x, y)$$

To make things simple, let $L_x = L_y = L$. Knowing the solutions to the 1D and 3D infinite potential wells,

(a) Propose a solution, $\psi(x, y)$ and E.

(b) What values are allowed for k_x and k_y? L

(c) Show that E only takes discrete values. Rewrite E using (b).

12. Determine the Fermi energy, E_f, for the free electron gas in 2D. You'll have to refer to results from the previous problem.

    (a) Plot the allowed energies in k-space. That is, make a graph with k_x on the horizontal and k_y on the vertical. Mark points or areas that correspond to allowed energy states.

    (b) Determine k_{max} or n_{max}, the radius of the quarter circle that encloses $N/2$ points. Use the area of a quarter circle.

    (c) Why do we use N/2, just half the number of free electrons?

    (d) Determine E_{f}, the highest filled energy. Use the result from problem 11c, and write this in terms of N.

13. Determine the density of states, $g(E) = dN/dE$, for the free electron gas in 2D. You'll have to refer to results from the previous problem.

    (a) Rewrite the result from 12c to be $N(E)$ (instead of $E(N)$).

    (b) Determine the density of states, $g(E)$.

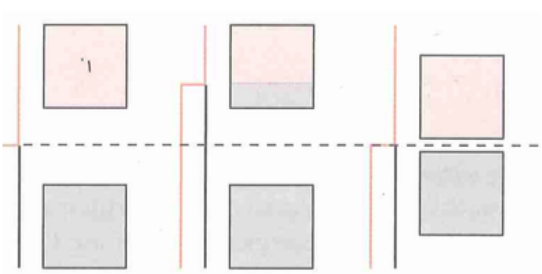
    (c) Describe, in words, what the density of states represents. Refer to a diagram.

---

14. (a) Determine the fermi energy E_F for sodium, gold, and aluminum. Give this in eV. You'll have to look up the density of valence electrons for each of these materials.

    (b) Calculate the Fermi velocity v_F in sodium, gold and aluminum. Give this in m/s.

15. The energy band schematics below are for $T = 0$.



    (a) Identify E_F in each of these diagrams.

    (b) Which electrons have a velocity approx that of the Fermi velocity? Indicate these on the schematics.

16. Determine the width of the "soft zone" of the F-D distribution at 300K. Let's say that this zone corresponds to the $f(E) = 0.9 \rightarrow 0.1$

    (a) Calculate the energy at which $f(E) = 0.9$. To make things simpler, calculate $E - E_F$.

    (b) Repeat for $f(E) = 0.1$.

    (c) Determine the width from (a) and (b).

    (d) Calculate the width of the soft zone at 300K. Give this in eV. For reference, sodium has a fermi energy of 3.22eV.

    ($4.4k_BT$, 0.10eV)

17. It's only the electrons in the soft zone that can participate in electrical or thermal conduction. Why?

18. The number of electrons that have an energy between E and $(E + \Delta E)$ is

$$N = \int_{E}^{E+\Delta E} g(E)f(E,T)dE$$

    You can think of this as

$$= \sum_{\text{E}_\text{i}} (\#\text{ states at E}_\text{i}) \times (\text{probability E}_\text{i}\text{ occupied})$$

    (a) Sketch the following graphs: $g(E)$, $f(E,T)$, and $g(E)f(E,T)$. On the $g(E)f(E,T)$ graph, indicate which electrons can participate in thermal and electrical conduction.

    (b) Estimate the integral by calculating the area of a simple triangle. The triangle's base is your result from 16c. The height is $g(E_F)$. Determine an expression for N. [You're working towards $N = 2k_bT(\frac{V}{2\pi^2})(\frac{2m_e}{\hbar^2})^{\frac{3}{2}}E_f^{1/2}$]

    (c) From the above, calculate the density of participating electrons, N/V, for sodium which has a Fermi energy of 3.22eV.

    (d) Compare the number of participating electrons to all the valence electrons. For sodium, $n_{\text{valence}} = 2.65 \times 10^{28}$.

    (6.5×10^{26}, 2.5%)

19. At a high enough temperature, an appreciable fraction of electrons are excited above E_F. This temperature is called the Fermi temperature T_F, and is given by $E_F = k_BT_F$.

    (a) Calculate the Fermi temperature for sodium, gold and aluminum.

    (b) Compare these temperatures to our sun's surface temperature of 5800K.
