8 Exam Question V2022

1. Quantum mechanical model of electrons in solids: free electron gas (30p)

   (a) Describe most important assumptions used to derive the quantum mechanical free electron gas model.

   Answer: 3D potential energy well; electrons are constrained within the volume of the metal with a potential energy barrier at the boundary (3D potential energy well). Electrons are otherwise free to move inside the metal (like an ideal gas) and do not interact with each other. No potential energy is associated with interactions between electrons and the atomic cores (positive ions in the crystal lattice). Only valence electrons that are weakly bound will form the free electron gas (metallic bond model). Quantization of energy is not a assumption but a results of confinement. Electrons are treated as fermions, this requires that no two electrons are found in the same quantum state. A classical free electron gas obeys Maxwell–Boltzmann statistics in which all electrons can have the same energy at 0 K, this is clearly not in agreement with the exclusion principle. As a consequence, even at zero temperature, some electrons have significant energy and significant velocity, Fermi energy and Fermi velocity.

   (b) Consider Lithium metal. For an alkali metal, one normally assumes that one electron per atom is "free" to travel within the sample (i.e. one electron per atom is delocalised and contributes to the metallic bonding and the electrical conductivity).

   What is the reason for this assumption?

   Answer: The charge distribution seen by the outer electron is very much like that seen by the electron in a hydrogen atom. The electron experiences a spherically symmetric central field due to presence of the closed 1s shell. The excited energy levels of the outer 2s electron are compared with those of hydrogen. The 2s electron in a Li atom is less strongly bound than any of the electrons in inner fully filled subshells. Its binding energy is comparable to that of the electron in the hydrogen atom. Formation of a metalic bond (delocalization) reduces the energy of the electron.

   (c) Imagine that we have a chain of Li atoms of length 1 cm. How many atoms (and how many delocalised electrons) does it contain?

   Answer: Using atomic radius $r = 152\,\mathrm{pm}$

   $$N = \frac{l}{2r} = \frac{1 \times 10^{-2}\,\mathrm{m}}{2 \cdot 1.52 \times 10^{-10}\,\mathrm{m}} = 3.3 \times 10^{7}$$

   (d) Assuming that T = 0 K, what is the energy of the highest occupied state (i.e. the Fermi energy) for this 1D system?

   Answer: Free electron gas for this 1D system will contain N electrons and $N/2$ energy levels. From this we can calculate the Fermi Energy:

   $$\begin{aligned} E_1 &= \frac{\hbar^2\pi^2}{2m_e a^2} = 6.0 \times 10^{-34}\,\mathrm{J} = 3.8 \times 10^{-15}\,\mathrm{eV} \\ E_F &= \left(\frac{N}{2}\right)^2 E_1 = 3.8 \times 10^{-15}\,\mathrm{eV} \cdot 3.3 \times 10^{7} \approx 1\,\mathrm{eV} \end{aligned}$$

(e) What is the Fermi velocity for electrons in this 1D system? What is the energy separation of the states at the Fermi energy? Is this consistent with it being a metal at room temperature?

Answer:

$$|v_F| = \sqrt{\frac{2E_F}{m}} = 6.0 \times 10^5\,\mathrm{m\,s^{-1}}$$

$$\begin{aligned} N_F &= N/2 \\ \Delta E &= (N_F+1)^2 E_1 - N_F^2 E_1 \approx 2N_F E_1 = 1.1 \times 10^{-14}\,\mathrm{eV} \end{aligned}$$

$\Delta E \ll k_B T$ which would support the hypothesis that this material can conduct electrical current.

(f) One of the most powerful applications of nanoscience is to be able to make structures such that the material properties are exactly what we want for a certain application.

Imagine that you want to make an 3D object with a shape of a cube, which is metallic at 100°C, but poorly conducting at room temperature. If you should make it from lithium, what size should it be?

Answer: The size can be estimated by assuming that ΔE at the Fermi level is $\Delta E \approx k_B T$ for 100 °C. For 3D

$$\begin{aligned} N_F &= \left[\frac{3n_e a^3}{\pi}\right]^{\frac{1}{3}} \\ \Delta E &= 2N_F E_1 \\ \Delta E &= 2 \cdot \frac{\hbar^2\pi^2}{2m_e a^2}\left[\frac{3n_e a^3}{\pi}\right]^{\frac{1}{3}} = \frac{\hbar^2\pi^2}{m_e a}\left[\frac{3n_e}{\pi}\right]^{\frac{1}{3}} \\ a &= \frac{\hbar^2\pi^2}{m_e \Delta E}\left[\frac{3n_e}{\pi}\right]^{\frac{1}{3}} \end{aligned}$$

where n_e is the concentration of charge carriers in e/m^3. For lithium,

$$\begin{aligned} n_e = 534\,\mathrm{kg\,m^{-3}} \cdot \frac{1}{6.94 \times 10^{-3}\,\mathrm{kg\,mol^{-1}}} &= \\ = 7.6 \times 10^4\,\mathrm{mol\,m^{-3}} = 4 \times 10^{28}\,\mathrm{e/m^3} \end{aligned}$$

$$a = \frac{\hbar^2\pi^2}{m_e \Delta E}\left[\frac{3n_e}{\pi}\right]^{\frac{1}{3}} = 79\,\mathrm{nm}$$

Useful constants: Density of crystalline Lithium : $\rho_{Li} = 0.534\,\mathrm{g\,cm^{-3}}$, Li atomic radius 152 pm. M_W=6.94 g mol^{-1} .

2. WAVES 1 (20p)

(a) Explain in what way, was the concept of standing waves important in the development of Bohr model of the hydrogen atom. What assumptions were needed. What were the main successes of the Bohr model? What did it fail to describe?

Answer: Some keywords: Bohr model of the hydrogen atom is bases on the classical planetary model, with a modification that the electrons can only exist on orbits with a particular radius. This radius corresponds to an integral number of de Broglie electron wavelengths along the allowed orbit and is equivalent to the statement that an electron orbit is allowed only if a de Broglie standing wave can form around its circumference. This is equivalent to the magnitude of the angular momentum, L, satisfies the equation

$$L = n\hbar$$

and we can show that this is equvalent to

$$n\lambda = 2\pi r$$

The model is able to predict Rydberg formula and allows to correctly calculate allowed energy levels for the electron in one-electron atom. Simplified, 1D approach that is not consistent with the three dimensional quantum mechanical analysis. Not possible to apply this model to more complex systems with more electrons. The theory gives no insights into important atomic properties such as line intensities.

(b) Why will a guitar string vibrate with only certain frequency/frequencies? Is it one or more? What physical parameters of the string are important to be able to predict the sound waved generated by such string? Explain and illustrate with drawings and equations.

Answer: Some keywords: 1D standing waves created by the interference between waves moving in the oposit directions along the string. Nodes at the ends of the string are required, as the string is fixed and can not oscillate at these points. This puts a constraint on the allowed wavelengths, and as a consequence allowed frequencies of the standing waves. Wave velocity if the function of tension applied to the string (T), as well as string's mass per unit length (μ).

$$v = \sqrt{\frac{T}{\mu}}$$

and

$$v = f\lambda$$

This can be used to show that allowed frequencies f_n are given by

$$f_n = \frac{nv}{2l}$$

where l is the length of the string and v is wave velocity.

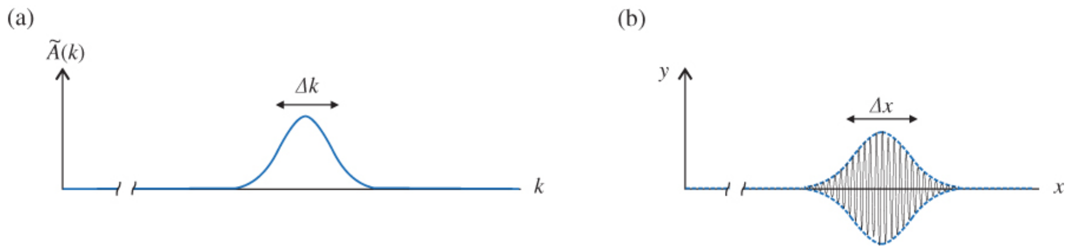
(c) What is defined by the term "wave packet". Illustrate with drawings, considering both frequency and spatial/time domains.

Answer: Wave pulse created by interference/superosition of many waves. One can show using Fourier analysis, that to create wave pulse, we must superpose sinusoidal waves with a continuous range of wave numbers. The Fourier analysis can be used to show that the width of the wavenumber spectrum, and the width of the wave packet, are related

$$\Delta k \Delta x \geq \frac{1}{2}$$

Similar analysis in the time domain connects range of frequency used to crate a wave pulse (wave packet) and the pulse duration.

$$\Delta\omega\Delta t \geq \frac{1}{2}$$



3. WAVES 2 (30p)

   (a) A model airplane is flying with a velocity of $20\,\mathrm{m\,s^{-1}}$ towards a wall. An observer is located 2000m from that wall and can hear the sound that comes directly from the airplane and the sound that is reflected from the wall. If the airplane motor generates a sound with a frequency of 1000 Hz, what frequencies will be heard by the observer assuming that there is no interference between direct and reflected waves. Speed of sound: $343\,\mathrm{m\,s^{-1}}$.

   Answer: Note: One need to assume that the airplane is between the observer and the wall or that the plane is further away from the wall than the observer and moves towards the wall. In the first case, two waves that reach the observer propagate in the same direction (away from the wall), and have different frequency given by the Dopler effect. Interference of these two waves will result in "beats" - amplitude that changes with time with a frequency that is $\omega_b = \frac{\Delta\omega}{2}$. If the plane is further away from the wall than the observer, wave that originates from the plane and the reflected wave have **the same frequency** but different propagation directions. This situation would result in interference that generates a standing wave. But since the plane is moving, that standing wave will not have the nodes, anti-nodes in a constant position, but these will change as a function of time. f_1 is the frequency of the wave generated in front of the plane (also the frequency of the reflected wave); f_2 is the frequency of the wave detected by the observer once the airplane is moving away from the observer.

$$f_1 = f_0 \frac{v}{v - v_{\text{source}}} = 1000\,\text{Hz} \frac{343}{343 - 20} = 1061\,\text{Hz}$$
$$f_2 = f_0 \frac{v}{v + v_{\text{source}}} = 1000\,\text{Hz} \frac{343}{343 + 20} = 945\,\text{Hz}$$

   (b) What will change if we assume that there is interference between the direct wave and the reflected wave? Can you derive a formula that will describe the amplitude of the sound wave that can be heard by the observer? Assume that sound velocity is constant and does not depend on the sound frequency.

   Answer: See above. Calculations that predict/illustrate beats due to interference of two waves moving in the same direction or a more complicated standing waves are necessary for the full score. Possible results are included below. Beats:

$$y = 2A\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)\sin(kx - \omega t + \phi)$$

Where, $\Delta\omega$ is the angular frequency difference between forward and backward waves. Solution that is a standing wave:

$$y = 2A\sin(kx + \phi(t))\cos(\omega t)$$

where $\phi(t)$ would be a time-dependent phase shift that depends on the position of the airplane at time t.

4. Answer one of the questions below (20p)

   (a) Explain reasons for the diffraction limit in a optical system.
   Answer: See textbook, section 22.3 (Diffraction at a single slit).

   (b) Outline Planck's theory of Black body radiation
   Answer: See textbook, section 14.2

   (c) What is the photoelectric effect and in what way was it important in the development of quantum mechanics.
   Answer: See textbook, section 14.5

   (d) What is a diffraction grating? Derive formula that allows you to calculate wave intensity after it has passed through such grating.
   Answer: See textbook, section 22.5