8 Exam Question V2021

1. Quantum mechanical model of electrons in solids: free electron gas

   (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. 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.

   (b) What properties of materials can this model describe?

   Answer: Quantised energy levels; Electrons occupied available energy levels in order of increasing energy - consequence of Pauli exclusion principle. Electrons are not in the ground (lowest energy state) even at 0K. Model allows us to calculate density of states, Fermi level and Fermi energy, electron energy distribution at 0 K and at T > 0K. Correctly describes electronic heat capacity, electronic conductivity and it's temperature dependence. Response of the electrons to a applied electric field.

   (c) Equation below contains parameter a which has units of length. What is described by this parameter? What is the meaning of n here? What are E and E_1?

$$E = (n_x^2 + n_y^2 + n_z^2)E_1$$

$$E_1 = \frac{\hbar^2\pi^2}{2ma^2}$$

   Answer: QM free electron gas model treats the metal as a single bound system of fermions and a is the macroscopic size of the solid (the size of the potential energy well). n_i are quantum numbers that correspond to each degree of freedom for the electrons and we can write

$$E = n^2 E_1$$

   where

$$n^2 = n_x^2 + n_y^2 + n_z^2$$

   n describe the total energy E of a quantum state according to the equation above. $3E_1$ is the lowest allowed energy level for electrons in a solid with a volume of a^3 and in which the electrons are described by the QM free electron models.

   (d) What is described by parameter E_F, the Fermi energy? How is it connected to the equations in the previous question (Q1.3)?

   Answer: Highest occupied energy level at 0K in a free electron gas model. In a metallic solid, each atom will donate certain number of electrons to the free electron gas. The quantum state of these electrons are distributed over available states according to Pauli principle. We fill the states starting from the lowest energy level. Each level can accommodate certain number of electrons

(unique combination of n_x n_y n_z that results in n), Energy level of the last electron with the highest energy corresponds to E_F and

$$E_F = n_F^2 E_1$$

. n_F is connected to the size of the solid and electron density through:

$$n_F = \left(\frac{3n_e a^3}{\pi}\right)^{1/3}$$

(e) A gold crystal has an fcc lattice (unit cell has a cubic shape) a lattice constant of 4.08 Å and 4 gold atoms in the unit cell. Each gold atom donates one electron to the free electron gas. Calculate the electron number density, Fermi energy, Fermi velocity and electron wavelength in a gold crystal.
Answer: $n = 5.89 \times 10^{28}\,\mathrm{m}^{-3}$ $E_F = 8.8 \times 10^{-19}\,\mathrm{J}$ $v_F = 1.4 \times 10^{6}\,\mathrm{m\,s}^{-1}$

$$\lambda_F = \frac{h}{p} \approx \frac{h}{mv_F} \approx 5 \times 10^{-10}\,\mathrm{m}$$

(f) What aspects of electron behaviour in solid materials are not captured by the free electron gas model.
Answer: Interactions between electrons and a periodic potential energy field from the ions; As a consequence FEG model does not predict electronic bands; there is no upper limit of the energy levels that can be occupied by the electrons and energy states are semi-continuous for all values of energy above the ground state. The model can only describe metals, and can not be applied to other materials; does not predict positive charge carriers; band gap for semiconductors;

2. Standing waves

(a) What are standing waves? Give some examples.
Answer: Created by interference of 2 waves with the same frequency and constant phase difference that propagate in a opposite direction along a common axis in 1D (2D and 3D standing waves are also possible, for example in 2D, waves on a surface of a drum can form 2D standing waves). These can be transverse as for example a wave on string (guitar) or longitudinal as in a pipe filled with air (sound waves in a musical instrument like a flute). Waves are typically created by interference of incident and reflected waves that are produced by the same source.

(b) Design and describe an experiment in which you demonstrate the existence of standing waves. You can use couple of small speakers (size of 1cm) that generates sound with a frequency of 50Hz (connected to a single signal generator) and a small microphone (1mm) connected to a PC. Alternatively you can use a water tank with one or two wave-generating devices (Ripple tank) and a sensor that is able to measure water level height. Derive mathematical expression that describes the standing wave in your experiment and plot wave profile you expect to detect.
Hint: Two waves that are generated by sources that are in phase but are separated by a distance L can be described by:

$$y_1 = A\sin(kx - \omega t + \phi_0)$$

$$y_2 = A\sin(k(x-L) - \omega t + \phi_0)$$

Answer: When using 2 speakers, one would expect a standing wave between the speakers. For a frequency of 50 Hz, and using the speed of sound $v_S = 340\,\mathrm{m\,s^{-1}}$the wave length is

$$\lambda = v_s f = 6.8\,\mathrm{m}$$

If we are using two sources, the standing wave will form for any separation between the speakers.

$$\begin{aligned} y_1 &= A\sin(kx - \omega t) \\ y_2 &= A\sin(k(x-L) + \omega t) \\ y_2 &= A\sin(kx + \omega t + \phi) \end{aligned}$$

where $\phi = -kL$, L is the separation between sources and $k = \frac{2\pi}{\lambda}$. Note that in the equation above, the wave y_2 moves in a opposite direction to the first one (as a consequence of a different sign in front of the ωt term).

$$\begin{aligned} y = y1 + y2 = A\sin(kx - \omega t) + A\sin(kx + \omega t + \phi) = \\ = A\left[\sin(kx - \omega t) + \sin(kx + \omega t + \phi)\right] = \\ = 2\sin(kx + \phi/2)\cos(-\omega t - \phi/2) \end{aligned}$$

that gives a standing wave for any value of $L \neq 0$. The equation is only valid for x between (0, L) - in the region where the two waves move in a opposite directions. If we use reflection to generate the 2nd wave, we need to position the speaker (wave source) in a distance from the barrier from which the wave is reflected such that a node will be present at the barrier. After setting up speakers, we need to measure sound amplitude along the axis between the two speakers and show that both nodes and antinodes are present. For 50Hz, a large separation is needed ($L > \lambda$) to observe both nodes and antinodes.

(c) Understanding of standing waves is important in the design of musical instruments. Give some examples. What are harmonics in this context? Would a guitar sound differently when played on the space station? Would a flute sound differently inside a air-filled diving bell in which the pressure p is 4 atmospheres. Support your answers by calculations.

Answer: Standing waves give raise to well defined frequencies that can be generated in a musical instrument. Fundamental frequency corresponds to the standing wave with the lowest possible frequency that can form resonance. For a string that is clamped on both ends, this will correspond to

$$f_1 = \frac{v}{2l} \quad \lambda_1 = 2l$$

Here, the wavelength in twice the string length. For higher harmonics, $\lambda = \frac{2l}{n}$. Wave with n=2 will have one node, wave with n=3 will have 2 nodes.

For guitar on the space station: wave velocity given by

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

where μ is the mass per unit length and T is tension. It is the mass and not weight, so the motion of the string will not be affected by gravity. The guitar will sound the same as on earth. Formula for sound velocity as a function of pressure for sound waves is (see textbook section 13.13).

$$v = \sqrt{\frac{\gamma P}{\rho}}$$

where γ is heat capacity ratio (the adiabatic index). So it appears that the velocity of sound depends on pressure P. But if the media obeys ideal gas law, the density will also depend on pressure and

$$v = \sqrt{\frac{\gamma kT}{\langle m \rangle}}$$

where $\langle m \rangle$ is the average molecular weight of the gas molecules. Therefore, the velocity of sound depends on the temperature but not on pressure. Assuming that ideal gas relation is sufficiently accurate for pressures between p_0 and $4p_0$ the conditions for resonance (frequency of the standing wave) will not change and the flute will sound the same.

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

If v is a function of pressure (ideal gas assumption does not hold), the frequency would change, but one would expect this effect to be small. Fun fact: if we on the other hand try to play the same instrument with helium, lower average molecular mass will result in higher velocity, and therefore higher frequency of the resonant modes.

(d) Are standing wave phenomena important in quantum mechanics or atomic physics? Explain and if they are, give some examples.

Answer: Bohr model of H-atom - standing waves along allowed orbits; particle in a box: allowed solutions for the wave function are standing waves in a 1D (2D or 3D) cavity. QM model of H-atom: wave functions are 3D standing waves - 2D analogy would be standing waves on a circular drum.

3. Propagating waves.

(a) A propagating sinusoidal wave can be described by the following equation:

$$y(x,t) = A\cos(\omega t - kx + \phi)$$

where $y(x,t)$ describes the amplitude at location and at time.

- The same wave can also be described using a complex notation. Introduce this notation.
- Use complex notation or the formula given above to derive a formula that can be used to calculate the distance between two points along the x-axis that oscillate in phase.

Answer:

$$y(x,t) = A\cos(kx - \omega t + \phi)$$
$$z(x,t) = Ae^{i(kx-\omega t+\phi)}$$
$$y(x,t) = \mathrm{Re}\left\{(z(x,t)\right\}$$

Two points that oscillate in phase along the wavefront:

$$z(x_1,t) = z(x_2,t)$$
$$Ae^{i(kx_2-\omega t+\phi)} = Ae^{i(kx_1-\omega t+\phi)}$$

The two equation are equal when:

$$kx_2 = kx_1 + 2\pi n$$
$$x_2 - x_1 = \Delta x = 2\pi n\frac{1}{k} = 2\pi n\frac{\lambda}{2\pi}$$
$$\Delta x = n\lambda$$

(b) Consider a one-dimensional system with two independent and identical wave sources: S1 located at $x = 0$ and S2 at $x = \Delta x$. Derive the expression for time-dependent amplitude at a observation point O located at the distance x_0 from S1. Consider only situations where $x_0 > \Delta x$. Plot amplitude at as the function of the separation distance between sources Δx

Answer: Disturbance at point O will be described by

$$z(x_0,t) = Ae^{i(kx_0-\omega t+\phi)} + Ae^{i(k(x_0-\Delta x)-\omega t+\phi)}$$

We can set $\phi = 0$, as this phase is the same for both waves. Below, we set $x = x_0$, as we are only interested in the amplitude at this value of x. More general derivation is also correct.

$$z(x_0,t) = Ae^{i(kx_0-\omega t)} + Ae^{i(k(x_0-\Delta x)-\omega t)}$$
$$y(x_0,t) = \mathrm{Re}\left\{(z(x_0,t)\right\}$$
$$z(x_0,t) = Ae^{i(kx_0-\omega t)} + Ae^{i(k(x_0-\Delta x)-\omega t)}$$
$$z(x_0,t) = Ae^{i(kx_0-\omega t+k\Delta x/2)}\left[e^{-ik\Delta x/2} + e^{ik\Delta x/2}\right]$$
$$z(x_0,t) = Ae^{i(kx_0-\omega t+k\Delta x/2)}2\cos\left(k\Delta x/2\right)$$
$$z(x_0,t) = 2A\cos\left(k\Delta x/2\right)e^{i(kx_0-\omega t+\phi)}$$
$$z(x_0,t) = 2A\cos\left(k\Delta x/2\right)e^{i(kx_0-\omega t+\phi)}$$
$$y(x_0,t) = 2A\cos\left(k\Delta x/2\right)\cos(kx_0-\omega t+\phi)$$

Note: Writing the equation above as:

$$z(x_0,t) = Ae^{i(kx_0-\omega t)} + Ae^{i(k(x_0-\Delta x)-\omega t)} = Ae^{i(kx_0-\omega t)}\left[1 + e^{-i(k\Delta x)}\right]$$

and finding the absolute value of the term in the square bracket gives an incorrect answer. We have a product of two complex numbers, and one need first to express this as $re^{i\phi}$, where r is real-valued, before finding the correct expression for the amplitude.

The amplitude is given by the term $2A\cos(k\Delta x/2)$ and the phase of the resulting disturbance at x_0 will also depend on the value of Δx by

$$\phi = k\Delta x/2$$

The phase also depend on the value of x_0 (the distance between the observation point and the first source) with the kx_0 term in the time dependent cos function above. To verify, the equation above predicts constructive interference for

$$k\Delta x/2 = n\pi$$
$$\Delta x = 2\pi n\frac{1}{k} = 2\pi n\frac{\lambda}{2\pi} = n\lambda$$

4. You have made a line pattern in a thin metal film deposited on a glass substrate (see figure, line spacing is d and line width is a). You need to verify that this periodic structure has been fabricated correctly. You look around the lab, but the only instrument you find is a laser pointer, that uses green light with a wavelength λ= 550nm. You also have your phone with you and can use the phone camera. Explain how you would investigate this.

   Hint: What physical phenomena can you use to measure d and a? Can you estimate what range of sizes can be measured? Can both a and d be measured and can this be done in the same experiment? Support your answers by calculations.

   Answer: Diffraction grating condition for observed maxima is

   $$d\sin\theta_M = n\lambda$$

   where θ_M is the angle at which a maximum is observed. We can use this to calculate d which is the repeating distance of the slits with width a in the fabricated grating. The intensity of the maxima will be modulated by a more slowly varying diffraction envelope, in particular if the slit width a is much smaller then the repeating distance d. This envelope function will changes the intensity of diffraction maxima - single slit modulation. By locating missing or very weak maxima, one can estimate the shape of the single slit modulation function and therefore calculate slit width. This is more challenging than finding the periodicity of the diffraction grating. One could also do that by trying to select one slit from the grating and observe single slit diffraction. Single slit modulation:

   $$I(\alpha) \propto \left[\frac{\sin^2\alpha}{\alpha^2}\right]$$
   $$\alpha = \frac{\pi a}{\lambda}\sin\theta$$

5. Atomic Physics:

   (a) What steps and assumptions are necessary to use mater waves and time-independent Schrödinger equation to describe 1 electron atom like hydrogen? Why is the situation more complex for atoms that contain more than 1 electron?

   Answer: We need to define the potential energy function and into the SE. The potential energy function for the one-electron atom is the Coulomb potential $U(r)$ for a spherically symmetric system with a positive charge in the center. We need to define the effective mass of the electron, due to the fact that the center of mass of the system is not located exactly at the center of the nucleus. We now solve the time-independent SE (potential energy does not depend on

time). We apply a technique of variables separation in spherical coordinates and get one electron atom eigenfunctions (wave functions that are a solution of the SE equation) as well as eigenvalues that correspond to the energy of the electron in various quantum states. To get an exact solution for a atom that contains more electrons, electron-electron interactions would need to be included and electron spin would need to be considered. Separation of variable is no longer possible and the solution can not be found analytically.

(b) What experimental observations can be used to verify prediction from the quantum mechanical model of the one-electron atom?

Answer: Energy levels can be calculated. These can be measured by looking at frequency of atomic emission lines - transitions between allowed quantum states. The hydrogen spectrum. This is also partially explained by semi-classical Bohr model of H-atom, but the Bohr model is not able to predict line intensity. Zeeman effect and splitting of energy levels in the magnetic field can also be predicted from QM model of H-atom.

(c) What aspects of the one-electron atom model can be used to describe multi-electron atoms?

Answer: Approximate solution for multielectron atoms. One can assume that core electrons are screening the coulomb interactions between valence electrons and the nucleus, modified potential can be used to find solution for the wave function for these electrons. One can also use H-atom like orbitals as a initial solution of the SE for a more complex systems and refine the solution using numerical methods.