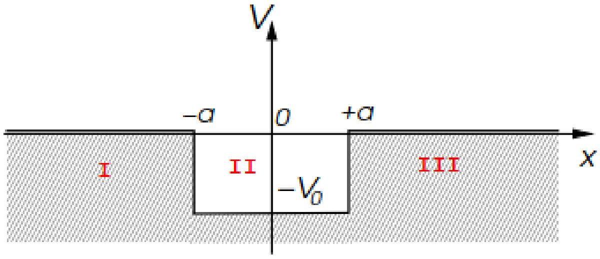
Semiconductors & Defects: Exercise 1 (02 Nov. '21)

General remark: Always try to come up with a short answer that catches the essence.

1. Calculation, schematic drawing, and discussion: Continuing from the explanations given on the blackboard, derive the solution for the energy of a quantum mechanical particle in a 1D box with finite barriers. Here is how far we got with this problem:



We are looking for the bound states of this potential; for their energy E it holds that $-V_0 < E < 0$. The Schrödinger equation in regions I and III can be written as $\psi''(x) - q^2\psi(x) = 0$, with $q^2 = \left|\frac{2mE}{\hbar^2}\right| > 0$, whereas in region II it can be written as $\psi''(x) + k^2\psi(x) = 0$, with $k^2 = \frac{2m(V_0+E)}{\hbar^2} > 0$. The wave function $\psi(x)$ and its first derivative need to be continuous at $x = \pm a$. So, we have four boundary conditions: $\psi_{\mathrm{I}}(-a) = \psi_{\mathrm{II}}(-a)$, $\psi'_{\mathrm{I}}(-a) = \psi'_{\mathrm{II}}(-a)$, $\psi_{\mathrm{II}}(a) = \psi_{\mathrm{III}}(a)$, and $\psi'_{\mathrm{II}}(a) = \psi'_{\mathrm{III}}(a)$. In addition, there is the normalization condition: $\int_{-\infty}^{\infty} |\psi(x)|^2\,\mathrm{d}x = 1$.

As an ansatz for the solution, regarding the mirror symmetry of the problem, one can use the following functions (other choices are also possible): For region III, the only possible solution is $\psi_{\mathrm{III}}(x) = A\mathrm{e}^{-qx}$, because the normalization condition requires $\psi(x \to \infty) \to 0$. Due to the symmetry, expressed as $\psi(-x) = \pm\psi(x)$, it follows that in region I, the solution is $\psi_{\mathrm{I}}(x) = \pm A\mathrm{e}^{qx}$; the relevant sign depends on the parity case under consideration, depending on the behavior in region II. In region II, the ungerade (odd parity) solution is $\psi_{\mathrm{II,u}}(x) = B\sin(kx)$, whereas the gerade (even parity) solution is $\psi_{\mathrm{II,g}}(x) = C\cos(kx)$.

Altogether, these functions contain five parameters (A, B, C, k, q), and there are five independent conditions to be fulfilled (one normalization and four boundary conditions). Therefore, there is a chance to find a solution. Note, however, that the relevant parameters, width and depth of the potential well, are not contained in A, B, and C, so we only need the solutions for k and q.

a) Derive the relevant equations which determine k and q. (Hints: Consider the cases of even and odd parity separately. These equations don't have analytic solutions). b) Discuss the possible solutions of these equations based on a graphical plot in the k–q plane. c) How do the energy levels of the bound states vary with respect to well width and well depth?

2. Formula, schematic drawing, and discussion: What is Bragg's condition for diffraction of X-rays from crystals? Why do we need the reciprocal space? What is the physical significance of Ewald's sphere?

3. Discussion and drawing: What is the special significance of the Brillouin Zones? Assuming a regular 1D chain of atoms, explain why an electron (treated in the nearly

free electron approximation) exhibits two energy values at $\boldsymbol{k} = \boldsymbol{k}_{\mathrm{BZ}}$ ($\boldsymbol{k}$: wave vector). Draw the $E(\boldsymbol{k})$ diagram for (i) the free electron gas and (ii) the free electron gas with diffraction at the first Brillouin zone edge. What is the advantage of the reduced zone scheme?

4. <u>Formula and discussion:</u> What is the Bloch theorem and its special significance for electrons in a crystal? For a Bloch wave, discuss the meaning of the "quasi wave vector" and the "crystal momentum."

5. <u>Schematic drawing and discussion:</u> Which fundamental information do we get about a semiconductor from its band structure?