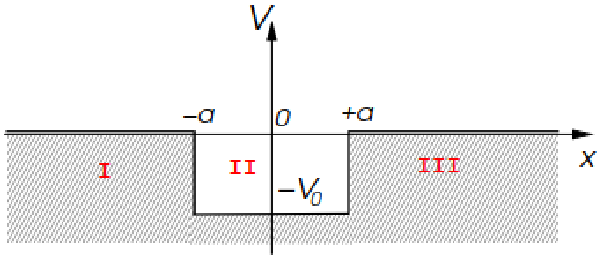
<u>Semiconductors & Defects: Exercise 1 (01 Nov. '22)</u>

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

1. <u>Calculation, schematic drawing, and discussion:</u> 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 in dependence on the box' width and depth.



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 are the normalization condition $\int_{-\infty}^{\infty} |\psi(x)|^2 \,\mathrm{d}x = 1$ ("there surely is a particle") and the mirror symmetry of the probability density, $|\psi(-x)|^2 = |\psi(x)|^2$. From the latter, we have a sign ambiguity for the wavefunction: $\psi(-x) = \pm\psi(x)$.

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 normalization condition requires $\psi(x \to \infty) \to 0$, so $\psi_{\mathrm{III}}(x) = A\mathrm{e}^{-qx}$ is the only possible solution. From the mirror symmetry we have that in region I the solution is $\psi_{\mathrm{I}}(x) = \pm A\mathrm{e}^{qx}$, the sign depending on the parity case under consideration which, in turn, depends on the behavior in region II. To go on, we now consider the parity in region II: The *ungerade* (odd parity) solution is $\psi_{\mathrm{II,u}}(x) = B\sin(kx)$, and the *gerade* (even parity) solution is $\psi_{\mathrm{II,g}}(x) = C\cos(kx)$; both lead to a symmetric probability density.

Altogether, we now have five parameters (A, B, C, k, q). For a given parity case, however, only four parameters enter the wave function (either the set A, B, k, q or the set A, C, k, q). Since there are only three conditions to be met (one normalization condition and two boundary conditions; the other two boundary conditions are equivalent by symmetry), there is a chance to find a multitude of solutions. Luckily, we only need the solutions for k and q, because only they contain the energy E that we are looking for. Therefore, the remaining task is just this:

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? (Hint: Use the graphical solution to discuss the variations just qualitatively.)

2. Formula and discussion: What are Bragg's and Laue's conditions for the 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 particle approximation) exhibits two energy values at $\boldsymbol{k} = \boldsymbol{k}_{\mathrm{BZ}}$ ($\boldsymbol{k}$: wave vector). Draw and discuss 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.

4. Formula and discussion: 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."