4 Electrons in a periodic potential (41 pts)

Due date: **Wednesday, 27th November 2024**.

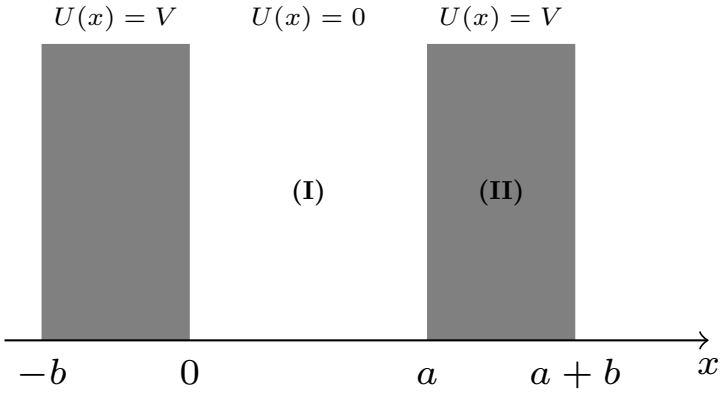
4.1 Concept of bands: 1D approximation of a crystal

Consider a one-dimensional crystal with the potential given by:

$$\forall x \in \cdots \quad \cup \quad [0, a[\quad \cup \quad [a+b, (a+b)+a[\quad \cup \cdots, \ U(x) = 0$$

$$\forall x \in \cdots \cup \quad [-b, 0[\quad \cup \quad [a, a+b[\quad \cup \quad [(a+b)+a, 2(a+b)[\quad \cup \cdots, \ U(x) = V > 0$$

periodically repeated over $N \gg 1$ periods of length $d \equiv a+b$. We use periodic boundary conditions. The x axis is therefore divided in zones, where the potential is either 0 or V. The region $[0, a]$ ($U(x) = 0$) is labeled region I, the region $[a, a+b]$ is labeled region II ($U(x) = V$).



(i) *(1 pt)* Give the expression for a wave function for a particle in this potential, using Bloch's theorem. The corresponding wave vector will be denoted k.

(ii) *(1 pt)* Give the general expressions for the solutions of the Schrödinger equation $\psi_I(x)$ and $\psi_{II}(x)$ for a particle of mass m, in region I and in region II respectively. These involve plane waves with wave vector k_1 and k_2 respectively, as well as two unknowns each, which will be denoted A, B for region I, C, D for region II. For simplicity, assume $E > V$, where E is the energy of the particle. Please pay attention to the specific domain of definition for each of the functions $\psi_I(x)$ and $\psi_{II}(x)$!

(iii) *(4 pts)* Use continuity constraints at points $x = 0$ and $x = a$ on the wave function, in order to obtain a set of four independent linear equations involving the unknowns introduced in the preceding question.

(iv) *(6 pts)* Show that the dispersion relation is given by:

$$\begin{aligned} \cos(k_1 a)\cos(k_2 b) - \frac{k_1^2 + k_2^2}{2k_1 k_2}\sin(k_1 a)\sin(k_2 b) &= \cos(kd) \\ k_1^2 - k_2^2 &= \frac{2mV}{\hbar^2} \end{aligned} \tag{13}$$

This is not a difficult calculation, but it is long; you need to keep things organized.

(v) *(2 pts)* Deduce from the above the expression for the dispersion relation in the configuration where $E < V$. (Use the notation $\frac{\hbar^2 \varkappa^2}{2m} = V - E$, you do **not** need to repeat the derivation!).

(vi) *(5 pts)* Use $a = \frac{10\hbar}{\sqrt{2m}}$, $b = \frac{2\hbar}{\sqrt{2m}}$, and $V = 1$. Plot the the profile of the left hand side of the dispersion relation, as a function of E, for $0 < E < 7$. Provide me with a transcript of your code, explaining how it works. Comment on your results, in relation to the concept of bands in solids.

4.2 Band structure in a periodic potential

Consider a two dimensional square lattice, with periodic boundary conditions, and with the periodic potential given by

$$U(x,y) = -4V\cos\left(\frac{2\pi x}{a}\right)\cos\left(\frac{2\pi y}{a}\right),$$

where a is the lattice parameter and $V > 0$. In this problem, we explore the band structure near the point $(\frac{\pi}{a}, \frac{\pi}{a})$, i.e., the corner of the 1st BZ. In all questions, we assume that $V \ll (\hbar^2/2m)(\pi/a)^2$. The arguments used when solving the problem can also be used when discussing band structures of simple metals.

(i) *(1 pt)* Give a description of the reciprocal lattice.

(ii) *(2 pts)* Give the expression of the Fourier expansion of $U(\boldsymbol{r})$.

(iii) *(1 pt)* Explain in plain words what the statement $V \ll (\hbar^2/2m)(\pi/a)^2$ tells us about the system. In particular, explain why this allows us to look for solutions of the Schrödinger equation in the form

$$\psi(\boldsymbol{r}) = \sum_{\boldsymbol{k}\in\text{BVK conditions}} c_{\boldsymbol{k}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}}\,. \tag{14}$$

(iv) *(3 pts)* Derive the so-called *central equation*, that is, the Schrödinger equation in $\boldsymbol{k}$-space. This provides you with a relation between all the coefficients $c_{\boldsymbol{k}}$: for any vector $\boldsymbol{K}$ from the reciprocal lattice,

$$\left[\frac{\hbar^2}{2m}(\boldsymbol{k}-\boldsymbol{K})^2 - E\right]c_{\boldsymbol{k}-\boldsymbol{K}} + \sum_{\boldsymbol{K'}} U_{\boldsymbol{K'}-\boldsymbol{K}} c_{\boldsymbol{k}-\boldsymbol{K'}} = 0 \tag{15}$$

Hint: Substitute the solution in the form given in (iii) to Schrödinger equation.

(v) *(2 pts)* Show that this allows you to write the solutions of the Schrödinger equation in the form

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{K}} c_{\boldsymbol{k}-\boldsymbol{K}} \mathrm{e}^{i(\boldsymbol{k}-\boldsymbol{K})\cdot\boldsymbol{r}}\,, \tag{16}$$

where the sum runs over all reciprocal lattice vectors, and $\boldsymbol{k}$ is any vector in the first Brillouin zone.

For $\boldsymbol{k}$ close to $\left(\frac{\pi}{a}, \frac{\pi}{a}\right)$, only the four following coefficients in the expansion of $\psi_{\boldsymbol{k}}(\boldsymbol{r})$, Eq. (16) are non-negligible:

$$c_{\boldsymbol{k}-\boldsymbol{K}}, \quad \forall \boldsymbol{K} \in \left\{\begin{pmatrix}1\\1\end{pmatrix}, \begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}, \begin{pmatrix}0\\0\end{pmatrix}\right\},$$

in units of $\frac{2\pi}{a}$.

(vi) *(4 pts)* Solve the central equation for $\boldsymbol{k}$ close to $\left(\frac{\pi}{a}, \frac{\pi}{a}\right)$: calculate the perturbed energy levels $E(\boldsymbol{k})$.

4.3 Density of states from the tight-binding model

Consider a tight-binding model on a square lattice, whose band structure is given by (we assume the lattice parameter is $a = 1$ for simplicity)

$$\epsilon(\vec{\mathbf{k}}) = -2t\sum_i \cos(k_i), \tag{17}$$

where i runs over all dimensions. We consider lattices in dimensions $d = 1, 2, 3$, so that the density of states can be written in a general manner

$$D(\epsilon) = \frac{2}{L^d}\sum_{\vec{\mathbf{k}}} \delta(\epsilon - \epsilon_{\vec{\mathbf{k}}}) \tag{18}$$

(i) *(3 pts)* Compute analytically the expression for $D(\epsilon)$ for $d = 1$.

(ii) *(3 pts)* For $d = 2$, $d = 3$, use numerics. Plot the profiles of $D(\epsilon)$ for $d = 1$ (analytic and numerical results together), $d = 2$, $d = 3$. Provide me with a transcript of your code, which should implement the elementary summation in some form (do not use the "histogram" feature of some numerical libraries).

(iii) *(3 pts)* Discuss and commment your results.