Ex1326: Eigenstates of 1D periodic lattice, Bloch's theorem

Submitted by: Daniel Kaplan, Raz Idan, Dor Korn

1 Problem statement

Consider a particle, with mass m, placed in a periodic lattice – which has the structure (a, b) (see diagram, below), and the hopping amplitudes between sites are c_a, c_b.

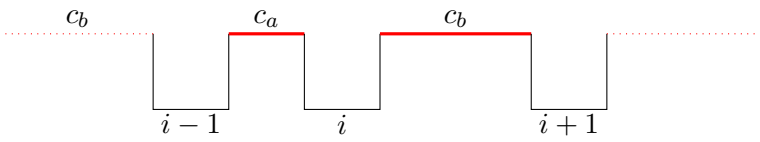
1. Construct the Hamiltonian matrix, assuming all sites have the same binding energy;
2. Define the displacement operator $\hat{D}$, with which $\hat{\mathcal{H}}$ commutes;
3. Find the two eigenstates of $\hat{\mathcal{H}}$ with periodicity $e^{-i\varphi}$.

Hint: the requested wavefunction is fully determined by two amplitudes (ψ_1, ψ_2) for which you should write a reduced eigen-equation.

4. Use the same procedure to find the eigen-equation for a lattice with the structure (a, a, b). Explain in what sense the reduced eigen-equation describes a ring.

2 Solution

With the information at hand, we visualize the lattice as a set of infinite points, as pictured in the diagram below. Without loss of generality, we will focus on a particular section, as shown. The sites are interspersed such that there are **2** sites per primitive cell.



2.1 The Eigenproblem

In order to construct the Hamiltonian in the general case, we exploit the inherent symmetry of the problem. Bloch's theorem dictates that by translating a **periodic** wavefunction, by exactly one period, we accumulate a phase factor. In this case, the period is **2**; the number of sites per cell. This is defined by a translation operator, displacing a wavefunction by that period, as:

$$\hat{D}(2) \cdot |\psi\rangle = e^{-i\varphi} |\psi\rangle \tag{1}$$

Since the eigenstates are unchanged by $\hat{D}$, we conclude:

$$\left[\hat{\mathcal{H}}, \hat{D}(2)\right] = 0 \tag{2}$$

The eigen-equation for the energies is defined:

$$\hat{\mathcal{H}} |\psi\rangle = E |\psi\rangle \tag{3}$$

By discretizing the wavefunction of the particle $|\psi\rangle \mapsto (\psi_1, \psi_2, \psi_3, \cdots)$ according to the sites, we may consider the energy balance for an arbitrary, i-th site. This will consist of the on-site energy (binding energy) and the transition amplitudes to neighboring sites. Thus:

$$\underbrace{\epsilon\psi_i}_{\text{On site E}} + \underbrace{c_a\psi_{i-1}}_{\text{Hopping from site i-1}} + \underbrace{c_b\psi_{i+1}}_{\text{Hopping from site i+1}} = E\psi_i \tag{4}$$

By deriving a similar expression for an adjacent site (see illustration, above), and recalling that in the discrete regime the periodicity depends on the number of sites in the repeating unit – 2 – and therefore $\psi_{i+2} = e^{-i\varphi}\psi_i$, we find:

$$\begin{aligned} \epsilon\psi_i + c_a\psi_{i-1} + c_b\psi_{i+1} &= E\psi_i \\ \epsilon\psi_{i+1} + c_b\psi_i + c_a\psi_{i+2} &= E\psi_{i+1} \end{aligned} \tag{5}$$

$$\Downarrow$$

$$\begin{aligned} \epsilon\psi_i + c_a\psi_{i-1} + c_b\psi_{i-1}e^{-i\varphi} &= E\psi_i \\ \epsilon\psi_{i-1}e^{-i\varphi} + c_b\psi_i + c_a\psi_i e^{-i\varphi} &= E\psi_{i-1}e^{-i\varphi} \end{aligned} \tag{6}$$

The above system is fully determined, as indicated by the number of independent variables. This provides a two-dimensional eigen-system, from a previously infinite element matrix. If we set, for simplicity $(\psi_{i-1}, \psi_i) = (\psi_1, \psi_2)$, we can rewrite the above as follows:

$$\underbrace{\begin{pmatrix} \epsilon & c_a + c_b e^{i\varphi} \\ c_a + c_b e^{-i\varphi} & \epsilon \end{pmatrix}}_{\tilde{\mathcal{H}}} \cdot \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \tag{7}$$

We instantly see that $\tilde{\mathcal{H}} = \tilde{\mathcal{H}}^\dagger$ as constrained by physical considerations. The Eigenvalues of $\tilde{\mathcal{H}}$ are readily obtained, granting:

$$E_\pm = \epsilon \pm \sqrt{c_a^2 + c_b^2 + 2c_a c_b \cos(\varphi)} \tag{8}$$

And the eignevectors:

$$\begin{aligned} \psi_+ &= \left(\tfrac{E_+ - \epsilon}{c_a + c_b e^{-i\varphi}}, 1\right) \\ \psi_- &= \left(\tfrac{E_- - \epsilon}{c_a + c_b e^{-i\varphi}}, 1\right) \end{aligned} \tag{9}$$

Thus, we have found the eigenstates of the problem.

3 The (a,a,b) case

If we consider the case of a lattice structured (a, a, b), we can reuse the above manipulation, to find the following set of equations:

$$\begin{aligned} \epsilon\psi_i + c_a\psi_{i-1} + c_a\psi_{i+1} &= E\psi_i \\ \epsilon\psi_{i+1} + c_a\psi_i + c_b\psi_{i+2} &= E\psi_{i+1} \\ \epsilon\psi_{i+2} + c_b\psi_{i+1} + c_a\psi_{i+3} &= E\psi_{i+2} \end{aligned} \tag{10}$$

We observe, however, that for such a configuration, the number of sites per repeating unit is now 3 – as determined by the lattice structure. Hence, we have for the periodicity in the discrete mode: $\psi_{i+3} = e^{-i\varphi}\psi_i$. Thus, the equations are transformed:

$$\begin{aligned} \epsilon\psi_i + c_a\psi_{i-1} + c_a\psi_{i+1} &= E\psi_i \\ \epsilon\psi_{i+1} + c_a\psi_i + c_b e^{-i\varphi}\psi_{i-1} &= E\psi_{i+1} \\ \epsilon e^{-i\varphi}\psi_{i-1} + c_b\psi_{i+1} + c_a e^{-i\varphi}\psi_i &= E e^{-i\varphi}\psi_{i-1} \end{aligned} \tag{11}$$

By setting the amplitude vector, as $(\psi_{i-1}, \psi_i, \psi_{i+1}) = (\psi_1, \psi_2, \psi_3)$, we obtain the eigen-equation:

$$\begin{pmatrix} \epsilon & c_a & c_b e^{i\varphi} \\ c_a & \epsilon & c_a \\ c_b e^{-i\varphi} & c_a & \epsilon \end{pmatrix} \cdot \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} \tag{12}$$

We see at once that this eigenvalue system describes a familiar problem: a ring in Aharonov-Bohm geometry such that flux (phase accretion per unit length) is present, and contained within the phase φ. The energy in the eigenproblem naturally depends on this phase, and will be altered accordingly.