Ex1327: Eigenstates of a 2D periodic lattice, Bloch theorem

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The problem:

Consider a particle in a 2D periodic square lattice. The lattice constant is a and consists of two sub-lattices. Accordingly the unit-cell is composed of two sites whose binding energy difference is ε. All the hoping amplitudes are c. Find the energy dispersion $E_{\pm}(\varphi_1, \varphi_2)$, where the φ's are the components of the Bloch quasi-momentum.

(1) Define translation operators (D_1, D_2) that generate the symmetry group of the lattice. This requires to identify principal axes.
(2) Write the wavefunction in terms of two amplitudes (ψ_A, ψ_B) given that it belongs to the (φ_1, φ_2) subspace of the symmetry group.
(3) Write the reduced 2x2 Hamiltonian within the (ψ_A, ψ_B) symmetry subspace.
(4) Find the eigen-energies $E_{\pm}(\varphi_1, \varphi_2)$
(5) Explain how your answer reduces to the usual expression for square lattice if $\varepsilon = 0$.

The solution:

(1) The lattice is symmetrical to diagonal translations as presented in figure 1. Therefore, translation operators that generate the symmetry group of the lattice can be defined as:

$$D_1\Psi = \mathrm{e}^{i\varphi_1}\Psi$$

$$D_2\Psi = \mathrm{e}^{i\varphi_2}\Psi$$

Where Ψ is an arbitrary wave function.
(In the context of solid state physics, the lattice is a Bravais lattice with a base spanned by the lattice vectors D_1 and D_2.)

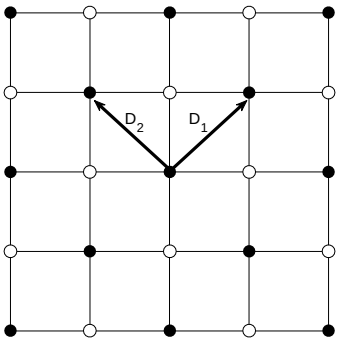

Figure 1: Lattice illustration. White sites are represented by ψ_A and black sites by ψ_B.

(2) A wave function in the subspace (φ_1, φ_2) can be represented as:

$$\Psi = \sum_{k,l,m,n} [D_1^k \cdot D_2^l]\psi_A + [D_1^m \cdot D_2^n]\psi_B$$

Where (ψ_A, ψ_B) represent the sites in an arbitrary unit cell (due to symmetry the location is insignificant). Without loss of generality we choose the on-site energy of ψ_A to be $\frac{\varepsilon}{2}$ and of ψ_B to be $-\frac{\varepsilon}{2}$.

(3) Hoping is allowed only between immediate neighbors with amplitude c.

$$\mathcal{H}\Psi = E\Psi$$

The Hamiltonian operation on each state can be derived by inspection of figure 2:

$$\begin{cases} E\psi_A = \frac{\varepsilon}{2}\psi_A + c[1 + \mathrm{e}^{i\varphi_1} + \mathrm{e}^{i\varphi_2} + \mathrm{e}^{i(\varphi_1+\varphi_2)}]\psi_B \\ E\psi_B = -\frac{\varepsilon}{2}\psi_B + c[1 + \mathrm{e}^{-i\varphi_1} + \mathrm{e}^{-i\varphi_2} + \mathrm{e}^{-i(\varphi_1+\varphi_2)}]\psi_A \end{cases}$$

Simplifying:

$$c[1 + \mathrm{e}^{\pm i\varphi_1} + \mathrm{e}^{\pm i\varphi_2} + \mathrm{e}^{\pm i(\varphi_1+\varphi_2)}] = c[(1 + \mathrm{e}^{\pm i\varphi_1})(1 + \mathrm{e}^{\pm i\varphi_2})] = \mathrm{e}^{\pm i\frac{\varphi_1+\varphi_2}{2}} 4c\cos(\frac{\varphi_1}{2})\cos(\frac{\varphi_2}{2})$$

Defining:

$$\eta = 4c\cos(\frac{\varphi_1}{2})\cos(\frac{\varphi_2}{2}) \quad , \quad \theta = \frac{\varphi_1 + \varphi_2}{2}$$

In matrix representation:

$$\mathcal{H} = \begin{pmatrix} \frac{\varepsilon}{2} & \mathrm{e}^{i\theta}\eta \\ \mathrm{e}^{-i\theta}\eta & -\frac{\varepsilon}{2} \end{pmatrix}$$

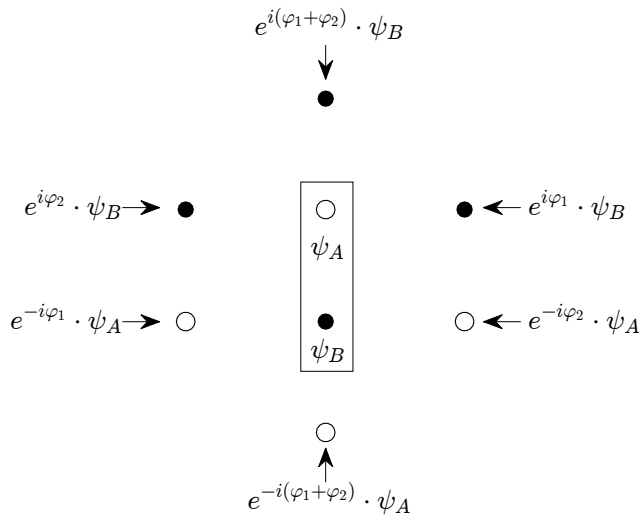

Figure 2: In the middle (ψ_A, ψ_B) form a unit cell. The sites surrounding the unit cell represent the neighbors map.

(4) The eigen-energies are:

$$E_\pm = \pm\sqrt{\eta^2 + \frac{\varepsilon^2}{4}}$$

(5) Having a square lattice with $\varepsilon = 0$ the translation operators which generate the group symmetry are one site translations in the x direction and in the y direction.

$$D_x\Psi = \mathrm{e}^{i\varphi_x}\Psi$$

$$D_y\Psi = \mathrm{e}^{i\varphi_y}\Psi$$

It is clear that:

$$\varphi_y = \frac{\varphi_1 + \varphi_2}{2} = \theta \quad , \quad \varphi_x = \frac{\varphi_1 - \varphi_2}{2}$$

There is a symmetry among all sites with exception of a phase. Hence, for an arbitrary site ψ:

$$E\psi = c(D_x + D_x^{-1} + D_y + D_y^{-1})\psi = c(\mathrm{e}^{i\varphi_x} + \mathrm{e}^{-i\varphi_x} + \mathrm{e}^{i\varphi_y} + \mathrm{e}^{-i\varphi_y})\psi$$

Simplifying:

$$E = 2c[\cos(\varphi_x) + \cos(\varphi_y)] = 4c\cos(\frac{\varphi_1}{2})\cos(\frac{\varphi_2}{2}) = \eta$$

We shall now show that the result of the previous problem reduces to the new one for $\varepsilon = 0$.
The new reduced Hamiltonian:

$$\mathcal{H}^* = \begin{pmatrix} 0 & \mathrm{e}^{i\theta}\eta \\ \mathrm{e}^{-i\theta}\eta & 0 \end{pmatrix}$$

$$E\begin{pmatrix}\psi_A \\ \psi_B\end{pmatrix} = \begin{pmatrix} 0 & \mathrm{e}^{i\theta}\eta \\ \mathrm{e}^{-i\theta}\eta & 0 \end{pmatrix}\begin{pmatrix}\psi_A \\ \psi_B\end{pmatrix} \quad (*)$$

Solving in order to find a relation between ψ_A and ψ_B we get: $\psi_A = \mathrm{e}^{i\theta}\psi_B$

Therefore, all sites are the same with exception of a phase, as expected, and the Hamiltonian can be reduced to a single element. By substitution of the relation between ψ_A and ψ_B into $(*)$, and solving the system of equations for E, we receive $E = \eta$.

The results are consistent.