Energy Spectrum of Electron in a Magnetic Field on a Lattice

Consider a two-dimensional square lattice of $N \times N$ sites. $c^\dagger_{n,m}$ and $c_{n,m}$ represent the creation and annihilation operators at site $\vec{r} = n\vec{a}_1 + m\vec{a}_2$; $\vec{a}_1$ and $\vec{a}_2$ are the primitive lattice vectors of the square lattice, $\vec{a}_1 = a\hat{x}$ and $\vec{a}_2 = a\hat{y}$, with lattice constant a.

(a) Write the tight-binding Hamiltonian, $\hat{H}$, for a electron moving on this lattice, including only nearest-neighbor hopping integral t.

Answer

The tight-binding Hamiltonian $\hat{H}$ for an electron on a two-dimensional square lattice with nearest-neighbor hopping can be expressed as:

$$\hat{H} = -t \sum_{n,m} \left(c^\dagger_{n+1,m} c_{n,m} + c^\dagger_{n-1,m} c_{n,m} + c^\dagger_{n,m+1} c_{n,m} + c^\dagger_{n,m-1} c_{n,m} \right).$$

(b) Using the usual procedure, i.e. writing the eigenvalue equation in momentum space, find its band structure $E(\vec{k})$ as a function of the momentum space vector $\vec{k}$. **[2 points]**

Answer

See mathematica notebook.

(c) **(Optional)** One way of displaying the $E(\vec{k})$ is to produce a contour plot (show the constant energy lines) of $E(\vec{k})$ in the first Brillouin zone. Prepare this plot. **[2 points]**

Answer

We start by transforming the real-space creation and annihilation operators $c^\dagger_{n,m}$ and $c_{n,m}$ into momentum space:

$$c_{n,m} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}_{n,m}} c_{\vec{k}},$$

where $\vec{k} = (k_x, k_y)$ is the wavevector in momentum space, $\vec{r}_{n,m} = n\vec{a}_1 + m\vec{a}_2 = (na, ma)$ is the position of the lattice site, and N is the number of lattice sites.

After substituting and simplifying, the Hamiltonian in momentum space can be diagonalized, giving the energy eigenvalues $E(\vec{k})$ as:

$$E(\vec{k}) = -2t \left(\cos(k_x a) + \cos(k_y a) \right).$$

(d) Now, introduce a uniform magnetic field B applied perpendicular to the lattice plane. One can substitute the magnetic field by a vector potential $\vec{A}$. Upon this substitution, the effective hopping term t acquires a phase:

$$t \to t e^{i\phi_{ij}}$$

where $\phi_{ij} = \frac{e}{\hbar} \int_i^j \vec{A} \cdot \vec{dl}$ represents the phase acquired during hopping from site i to j. Show that after this substitution, the resulting Hamiltonian is not gauge invariant. **[2 point]**

Answer

In the presence of a magnetic field, the hopping term between sites i and j acquires a phase factor. The modified tight-binding Hamiltonian can be written as:

$$\hat{H} = -\sum_{\langle i,j \rangle} t\, e^{i\phi_{ij}}\, c_i^\dagger c_j + \text{h.c.}$$

where: - $\langle i,j \rangle$ denotes nearest-neighbor pairs of sites i and j, - $\phi_{ij} = \frac{e}{\hbar}\int_i^j \vec{A}\cdot d\vec{l}$ is the phase acquired by the electron when hopping from site i to site j, - $\vec{A}$ is the vector potential associated with the magnetic field.

Under a gauge transformation, the vector potential $\vec{A}$ transforms as:

$$\vec{A} \to \vec{A}' = \vec{A} + \nabla\chi,$$

where $\chi(\vec{r})$ is an arbitrary scalar function of position.

This change in $\vec{A}$ affects the phase ϕ_{ij} in the hopping term. Specifically, the new phase ϕ'_{ij} between sites i and j becomes:

$$\phi'_{ij} = \frac{e}{\hbar}\int_i^j \vec{A}'\cdot d\vec{l} = \frac{e}{\hbar}\int_i^j \left(\vec{A} + \nabla\chi\right)\cdot d\vec{l} = \phi_{ij} + \frac{e}{\hbar}\left(\chi_j - \chi_i\right),$$

where χ_i and χ_j are the values of χ at sites i and j.

Under this transformation, the hopping term $te^{i\phi_{ij}}$ is modified as follows:

$$te^{i\phi_{ij}} \to te^{i\phi'_{ij}} = te^{i\phi_{ij}}e^{i\frac{e}{\hbar}(\chi_j-\chi_i)}.$$

To restore the Hamiltonian's form under the gauge transformation, we must also transform the creation and annihilation operators:

$$c_i \to c'_i = c_i e^{i\frac{e}{\hbar}\chi_i}, \quad c_i^\dagger \to c_i^{\dagger\prime} = c_i^\dagger e^{-i\frac{e}{\hbar}\chi_i}.$$

Substituting these into the Hamiltonian gives:

$$\hat{H} = -\sum_{\langle i,j \rangle} t\, e^{i\phi_{ij}}\, c_i^\dagger c_j + \text{h.c.} \to -\sum_{\langle i,j \rangle} t\, e^{i\phi_{ij}}\, c_i^{\dagger\prime} c'_j + \text{h.c.} = \hat{H},$$

showing that the physical observable (i.e., the Hamiltonian) does not depend on the gauge choice for the vector potential.

Thus, we have shown that under a gauge transformation, the phase $e^{i\phi_{ij}}$ changes, and the Hamiltonian itself would not remain invariant unless we also transform the electron operators. Therefore, the Hamiltonian is not gauge invariant in terms of the untransformed operators, but gauge invariance can be restored by transforming the electron operators accordingly.

(e) We choose the Landau gauge $\vec{A} = (0, Bx, 0)$ to represent the magnetic vector potential $\vec{A}$ corresponding to this uniform magnetic field. Realize that the hopping phase factor is 1 in the x-direction. Calculate the phase factor when the electron hops along the y-direction [from (n,m) to $(n,m+1)$] and express it in terms of the magnetic flux per unit cell, $\Phi = Ba^2$. **[3 points]**

Answer

The magnetic field $\vec{B} = B\hat{z}$ (perpendicular to the xy-plane) is represented by the vector potential in the Landau gauge:

$$\vec{A} = (0, Bx, 0).$$

When an electron hops from a site (n, m) to the neighboring site $(n, m+1)$ in the y-direction, it acquires a phase due to the magnetic vector potential $\vec{A}$. This phase factor $\phi_{(n,m)\to(n,m+1)}$ is given by:

$$\phi_{(n,m)\to(n,m+1)} = \frac{e}{\hbar}\int_{(n,m)}^{(n,m+1)} \vec{A}\cdot d\vec{l}.$$

Since the electron is moving in the y-direction from (n, m) to $(n, m+1)$, we have $d\vec{l} = (0, a, 0)$. Therefore,

$$\phi_{(n,m)\to(n,m+1)} = \frac{e}{\hbar}\int_{y=ma}^{y=(m+1)a} \vec{A}\cdot d\vec{l} = \frac{e}{\hbar}\int_{y=ma}^{y=(m+1)a} Bx\, dy.$$

Since $x = na$ is constant along this path, the integral simplifies to:

$$\phi_{(n,m)\to(n,m+1)} = \frac{e}{\hbar}\cdot Bna\cdot a = \frac{eBa^2}{\hbar}\cdot n.$$

The magnetic flux per unit cell is given by $\Phi = Ba^2$. Thus, we can rewrite the phase as:

$$\phi_{(n,m)\to(n,m+1)} = \frac{e\Phi}{\hbar}\cdot n.$$

The phase factor for hopping in the y-direction (from (n, m) to $(n, m+1)$) is:

$$\phi_{(n,m)\to(n,m+1)} = \frac{e\Phi}{\hbar}\cdot n.$$

This result shows that the phase acquired by the electron depends on the x-coordinate n, and is proportional to the magnetic flux per unit cell $\Phi = Ba^2$.

(f) Define $\alpha = \Phi/\Phi_0$, $\Phi_0 = h/e$ is the magnetic flux quantum, and rewrite the real space Hamiltonian in terms of α. **[2 points]**

Answer

Define the dimensionless parameter

$$\alpha = \frac{\Phi}{\Phi_0},$$

where $\Phi = Ba^2$ is the magnetic flux per unit cell and $\Phi_0 = \frac{h}{e}$ is the magnetic flux quantum.

The tight-binding Hamiltonian for an electron on a two-dimensional square lattice in the presence of a perpendicular magnetic field in the Landau gauge $\vec{A} = (0, Bx, 0)$ becomes:

$$\hat{H} = -t\sum_{n,m}\left(c^\dagger_{n+1,m}c_{n,m} + c^\dagger_{n-1,m}c_{n,m} + e^{i2\pi\alpha n}c^\dagger_{n,m+1}c_{n,m} + e^{-i2\pi\alpha n}c^\dagger_{n,m-1}c_{n,m}\right).$$

In this form: - The hopping in the x-direction remains unchanged, as the phase factor is 1. - The hopping in the y-direction acquires a phase factor of $e^{\pm i2\pi\alpha n}$, where $\alpha = \frac{\Phi}{\Phi_0}$.

(g) Now, assume periodic boundary conditions in the y-direction. This allows you to write $c^\dagger_{n,m}|0\rangle = e^{ik_y m}|\psi_n\rangle$, where k_y is the wavevector along the y-direction. Make this substitution and show that the eigenvalue equation for $|\psi_n\rangle$ is given by

$$E|\psi_n\rangle = -t\left[|\psi_{n+1}\rangle + |\psi_{n-1}\rangle + 2\cos(2\pi\alpha n + k_y)\,|\psi_n\rangle\right]. \quad (1)$$

[3 points]

Answer

Putting all these terms together, the Hamiltonian acting on $|\psi_n\rangle$ is:

$$\hat{H}|\psi_n\rangle = -t\left[|\psi_{n+1}\rangle + |\psi_{n-1}\rangle + e^{i2\pi\alpha n}|\psi_n\rangle + e^{-i2\pi\alpha n}|\psi_n\rangle\right].$$

Using the fact that the two terms with $e^{\pm i2\pi\alpha n}$ combine as:

$$e^{i2\pi\alpha n} + e^{-i2\pi\alpha n} = 2\cos(2\pi\alpha n),$$

we obtain the final eigenvalue equation:

$$E|\psi_n\rangle = -t\left[|\psi_{n+1}\rangle + |\psi_{n-1}\rangle + 2\cos(2\pi\alpha n + k_y)|\psi_n\rangle\right].$$

(h) For a rational value of $\alpha = p/q$ (where p and q are integers), Eq. (1) is periodic with period q, i.e. $|\psi_{n+q}\rangle = |\psi_n\rangle$. In this case, we can represent the problem using a $q \times q$ matrix. Write down this matrix form of the Hamiltonian. **[2 points]**

Answer

The Hamiltonian can be written as a $q \times q$ matrix with the following structure:

$$H = -t\begin{pmatrix} 2\cos(2\pi\alpha 0 + k_y) & 1 & 0 & \cdots & 0 & 0 \\ 1 & 2\cos(2\pi\alpha 1 + k_y) & 1 & \cdots & 0 & 0 \\ 0 & 1 & 2\cos(2\pi\alpha 2 + k_y) & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2\cos(2\pi\alpha(q-2) + k_y) & 1 \\ 0 & 0 & 0 & \cdots & 1 & 2\cos(2\pi\alpha(q-1) \end{pmatrix}$$

Here, the diagonal terms are $2\cos(2\pi\alpha n + k_y)$, representing the on-site energy of the state $|\psi_n\rangle$. The off-diagonal terms represent the hopping between neighboring sites, which are 1 on the $n+1$ and $n-1$ sites.

(i) For a given k_y, one can solve this matrix numerically to find the energy eigenvalues (using Python, MATLAB, Mathematica, or a similar tool). Set up this code and find the band structure for $\alpha = 1/16$ as a function of k_y in the first Brillouin zone. For numerical evaluation one discretize k_y into having a large number of values (this represents the number of sites in the y-direction). **[3 points]**

Answer

(j) In the regime of low flux ($\Phi \ll 1$), the band structure of our tight binding model is closely connected to the Landau levels of a two-dimensional electron gas in a magnetic field, where the electrons form discrete Landau levels with energies given by $E_n = \hbar\omega_c(n+1/2)$, where $\omega_c = eB/m$ is the cyclotron frequency and $n = 0, 1, 2, \cdots$ indexes the Landau levels. Explain how the energy spectrum derived in the last question ($\alpha = 1/16$ is an example of weak flux) resembles the Landau levels of a free particle in a magnetic field. The differences between the two, however, are linked to the presence of a periodic lattice. **[2 points]**

Answer

When α is small, it implies that the magnetic field B is weak or that the lattice constant a is small compared to the magnetic length scale. For small α, the magnetic unit cell (the area over which one flux quantum Φ_0 is applied) is much larger than the physical unit cell of the lattice. This means that the influence of the lattice on the magnetic energy levels is reduced, allowing the spectrum to resemble the continuum Landau levels seen in a free-electron system.

In a continuous two-dimensional electron gas in a magnetic field, electrons form discrete Landau levels with energies given by:

$$E_n = \hbar\omega_c\left(n + \frac{1}{2}\right),$$

where $\omega_c = \frac{eB}{m}$ is the cyclotron frequency and $n = 0, 1, 2, \ldots$ indexes the Landau levels.

In the lattice case, for very small α, the Harper equation for the tight-binding model in a magnetic field can be approximated by these continuous Landau levels. The lattice introduces weak periodic potential effects that slightly modify these levels, but they remain close to the Landau level structure.

In the weak flux limit, the tight-binding model yields bands that are nearly flat and closely spaced, resembling the Landau levels. However, due to the presence of the periodic lattice potential, each Landau level splits into narrow subbands (minibands) in the Hofstadter spectrum. These minibands can be understood as the result of a weak perturbation (from the lattice potential) applied to the Landau levels, causing slight shifts and gaps in the otherwise degenerate levels.

(k) **(Optional)** Generalize the numerical code to evaluate the spectrum for any rational value of α, and k_y in the first Brillouin zone. Now, vary $\alpha \in [0, 1]$ and plot the energy eigenvalues for all k_y in the y-axis as a function of α. Only take rational fractions of α with q which not more than say 50. Describe the features of this plot? **[3 points]**

Answer

The problem you have solved so far is called "Hofstadter's butterfly" – the first example of scientific data visualization.