

Magnetic Field in Lattice Model

Wangqian Miao
The Hong Kong University of Science and Technology

November 9, 2020

This note gives a more detailed derivation for the magnetic lattice symmetry part of *Di Xiao, Ming-Che Chang, and Qian Niu Rev. Mod. Phys. 82, 1959.*

1 Gauge Invariance

In quantum mechanics, the wavefunction should be necessarily different when we choose different gauge for the vector potential \mathbf{A} . The ‘Gauger Invariance’ states that

$$\begin{aligned}\mathbf{A} &\rightarrow \mathbf{A}' = \mathbf{A} + \nabla f \\ \psi &\rightarrow \psi' = \exp\left(-i \frac{ef}{\hbar}\right) \psi\end{aligned}\tag{1}$$

Here we let $c = 1$.

2 Magnetic Translation Symmetry

The single particle Hamiltonian after we apply a magnetic field should be:

$$H(\mathbf{r}) = \frac{1}{2m} [\mathbf{p} + e\mathbf{A}(\mathbf{r})]^2 + V(\mathbf{r})\tag{2}$$

Here we only concern about the system that the electrons are confined to $x - y$ plane and the magnetic field is uniform along the z axis. Since the original translational symmetry is broken by the vector potential $\mathbf{A}(\mathbf{r})$, we need to find the new translational symmetry of the system. Consider $H(\mathbf{r} + \mathbf{a})$, where \mathbf{a} is the lattice vector:

$$\begin{aligned}H(\mathbf{r} + \mathbf{a}) &= \frac{1}{2m} [\mathbf{p} + e\mathbf{A}(\mathbf{r} + \mathbf{a})]^2 + V(\mathbf{r} + \mathbf{a}) \\ &= \frac{1}{2m} [\mathbf{p} + e\mathbf{A}(\mathbf{r} + \mathbf{a})]^2 + V(\mathbf{r})\end{aligned}\tag{3}$$

The schodinger equation should be written as:

$$\left\{ \frac{1}{2m} [\mathbf{p} + e\mathbf{A}(\mathbf{r} + \mathbf{a})]^2 + V(\mathbf{r}) \right\} \psi(\mathbf{r} + \mathbf{a}) = E\psi(\mathbf{r} + \mathbf{a})\tag{4}$$

Then we take a navigation into \mathbf{A} , we define:

$$\Delta\mathbf{A}(\mathbf{a}) = \mathbf{A}(\mathbf{r} + \mathbf{a}) - \mathbf{A}(\mathbf{r}) = \nabla f\tag{5}$$

Here we should mention that a specific gauge should be specified (for most case, we use Landau gauge), as a result ΔA is independent of \mathbf{r} .

We can do the gauge transformation for the wavefunction ψ and it can help us remove $\Delta \mathbf{A}$ in the Hamiltonian:

$$\begin{aligned}\mathbf{A}(\mathbf{r} + \mathbf{a}) &\rightarrow \mathbf{A}(\mathbf{r}) = \mathbf{A}(\mathbf{r} + \mathbf{a}) - \nabla f \\ \psi(\mathbf{r} + \mathbf{a}) &\rightarrow \exp\left(i \frac{e}{\hbar} \Delta \mathbf{A}(\mathbf{a}) \cdot \mathbf{r}\right) \psi(\mathbf{r} + \mathbf{a})\end{aligned}\quad (6)$$

After gauge transformation, eq(4) should be written in the following way

$$\left\{ \frac{1}{2m} [\mathbf{p} + e\mathbf{A}(\mathbf{r})]^2 + V(\mathbf{r}) \right\} \exp\left(i \frac{e}{\hbar} \Delta \mathbf{A}(\mathbf{a}) \cdot \mathbf{r}\right) \psi(\mathbf{r} + \mathbf{a}) = E \exp\left(i \frac{e}{\hbar} \Delta \mathbf{A}(\mathbf{a}) \cdot \mathbf{r}\right) \psi(\mathbf{r} + \mathbf{a}) \quad (7)$$

We can define the Magnetic Translation Operator (MTO)

$$\hat{T}_{\mathbf{a}}^M \psi(\mathbf{r}) = \exp\left(i \frac{e}{\hbar} \Delta \mathbf{A}(\mathbf{a}) \cdot \mathbf{r}\right) \psi(\mathbf{r} + \mathbf{a}) \quad (8)$$

$[\hat{H}, \hat{T}_{\mathbf{a}}^M] = 0$ can be proved (from eq(7)):

$$\begin{aligned}\hat{H}(\mathbf{r}) \hat{T}_{\mathbf{a}}^M \psi(\mathbf{r}) &= \hat{H}(\mathbf{r}) \exp\left(i \frac{e}{\hbar} \Delta \mathbf{A}(\mathbf{a}) \cdot \mathbf{r}\right) \psi(\mathbf{r} + \mathbf{a}) = E \exp\left(i \frac{e}{\hbar} \Delta \mathbf{A}(\mathbf{a}) \cdot \mathbf{r}\right) \psi(\mathbf{r} + \mathbf{a}) \\ \hat{T}_{\mathbf{a}}^M \hat{H}(\mathbf{r}) \psi(\mathbf{r}) &= E \hat{T}_{\mathbf{a}}^M \psi(\mathbf{r}) = E \exp\left(i \frac{e}{\hbar} \Delta \mathbf{A}(\mathbf{a}) \cdot \mathbf{r}\right) \psi(\mathbf{r} + \mathbf{a})\end{aligned}\quad (9)$$

Magnetic translation operator along different directions usually do not commute. More commonly,

$$\begin{aligned}\hat{T}_{\mathbf{a}_i}^M \hat{T}_{\mathbf{a}_j}^M &= \hat{T}_{\mathbf{a}_j}^M \hat{T}_{\mathbf{a}_i}^M \exp\left(i \frac{e}{\hbar} \oint_{\mathcal{C}} \mathbf{A} d\mathbf{r}\right) \\ &= \hat{T}_{\mathbf{a}_j}^M \hat{T}_{\mathbf{a}_i}^M \exp\left(i \frac{e}{\hbar} \int B dS\right) \\ &= \hat{T}_{\mathbf{a}_j}^M \hat{T}_{\mathbf{a}_i}^M \exp\left(2\pi i \frac{\int B dS}{\Phi_0}\right)\end{aligned}\quad (10)$$

where $\Phi_0 = h/e$ is the flux quantum. \mathcal{C} is the contour of the cell defined by $\mathbf{a}_i, \mathbf{a}_j$. The above equation can be understood as Lattice AB Effect:

$$\hat{T}_{\mathbf{a}_i}^{M-1} \hat{T}_{\mathbf{a}_j}^{M-1} \hat{T}_{\mathbf{a}_i}^M \hat{T}_{\mathbf{a}_j}^M = \exp\left(i \frac{e}{\hbar} \oint_{\mathcal{C}} \mathbf{A} d\mathbf{r}\right) \quad (11)$$

3 Magnetic Unit Cell

Consider the following case (p, q are relatively prime):

$$\begin{aligned}\mathbf{a}_i &= \mathbf{a}_1, \mathbf{a}_j = q\mathbf{a}_2 \\ BS &= \frac{p}{q} \Phi_0 \\ \int B dS &= \frac{p}{q} \Phi_0 \times q = p\Phi_0\end{aligned}\quad (12)$$

where \mathcal{S} is the original unit cell size. As a result, we find three operators commute with each other:

$$[\hat{H}, \hat{T}_{\mathbf{a}_1}^M] = [\hat{H}, \hat{T}_{q\mathbf{a}_2}^M] = [\hat{T}_{\mathbf{a}_1}^M, \hat{T}_{q\mathbf{a}_2}^M] = 0 \quad (13)$$

The magnetic unit cell is q times larger than the original one with the unit lattice vector \mathbf{a}_1 and $q\mathbf{a}_2$.

4 Magnetic Bloch Theorem

By using the commutation relationship we can prove the magnetic bloch theorem (the proving process is the same as the original one, see page 132 from Solid State Physics, Hu An)

$$\begin{aligned} \hat{H}\psi_{n\mathbf{k}} &= E_{n\mathbf{k}}\psi_{n\mathbf{k}} \\ \hat{T}_{\mathbf{a}_1}^M\psi_{n\mathbf{k}} &= e^{i\mathbf{k}\cdot\mathbf{a}_1}\psi_{n\mathbf{k}} \\ \hat{T}_{q\mathbf{a}_2}^M\psi_{n\mathbf{k}} &= e^{i\mathbf{k}\cdot q\mathbf{a}_2}\psi_{n\mathbf{k}} \end{aligned} \quad (14)$$

What's more, the magnetic bloch condition should be:

$$\begin{aligned} \hat{T}_{\mathbf{a}_1}^M\psi_{n\mathbf{k}}(\mathbf{r}) &= e^{i\mathbf{k}\cdot\mathbf{a}_1}\psi_{n\mathbf{k}}(\mathbf{r}) = \exp\left(i\frac{e}{\hbar}\Delta\mathbf{A}(\mathbf{a}_1)\cdot\mathbf{r}\right)\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{a}_1) \\ \psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{a}_1) &= \exp\left(-i\frac{e}{\hbar}\Delta\mathbf{A}(\mathbf{a}_1)\cdot\mathbf{r}\right)e^{i\mathbf{k}\cdot\mathbf{a}_1}\psi_{n\mathbf{k}}(\mathbf{r}) \end{aligned} \quad (15)$$