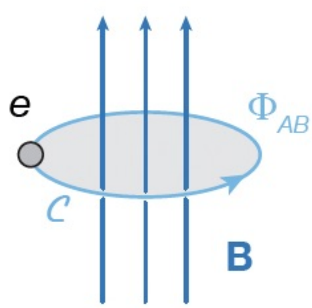
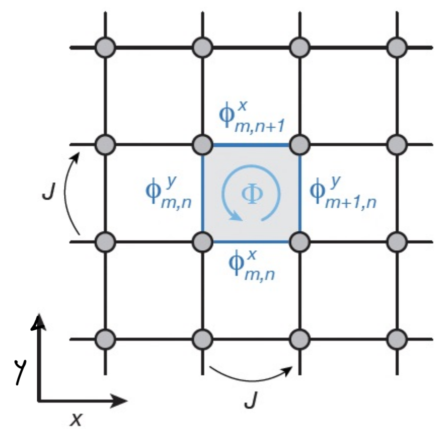
II. Hofstadter model

1 Charged particles on a lattice in the presence of a magnetic field – Peierls substitution

Reminder: Aharonov Bohm



lattice $\Longrightarrow$



Lattice

Complex tunneling matrix elements with Peierls phases

$$\phi^i_{m,n} , \quad i = \{x,y\} ; \qquad \phi^x_{m,n} = -\frac{e}{\hbar} \int_m^{m+1} A_x(x,n)\, dx$$

$\Rightarrow$ Aharonov–Bohm phase around one unit cell (plaquette)

$$\boxed{\Phi = \phi^x_{m,n} + \phi^y_{m+1,n} - \phi^x_{m,n+1} - \phi^y_{m,n}}$$

which is related to the vector potential $\vec{A}$

$$\boxed{\Phi_{AB} = -\frac{e}{\hbar} \oint_C \vec{A} \cdot d\vec{r} = -2\pi \, \Phi_B / \Phi_0}$$

where Φ_B is the magnetic flux and $\Phi_0 = h/e$ is the magnetic flux quantum, which is often denoted as $\boxed{\alpha = \Phi_B / \Phi_0 = \Phi/(2\pi)}$

Tight-binding Hamiltonian

$$\boxed{\hat{H} = -J \sum_{m,n} \left(e^{i\phi^x_{mn}} \hat{a}^\dagger_{m+1,n} \hat{a}_{m,n} + e^{i\phi^y_{m,n}} \hat{a}^\dagger_{m,n+1} \hat{a}_{m,n} + h.c. \right)}$$

How to solve this problem?

For zero magn. flux $\Phi = 0$:

$\rightarrow$ lattice translation operators commute with the Hamiltonian and they commute with each other

$\Rightarrow$ Bloch theorem

Translation operators: $$\hat{T}^0_x = \sum_{m,n} \hat{a}^\dagger_{m+1,n} \hat{a}_{m,n}$$

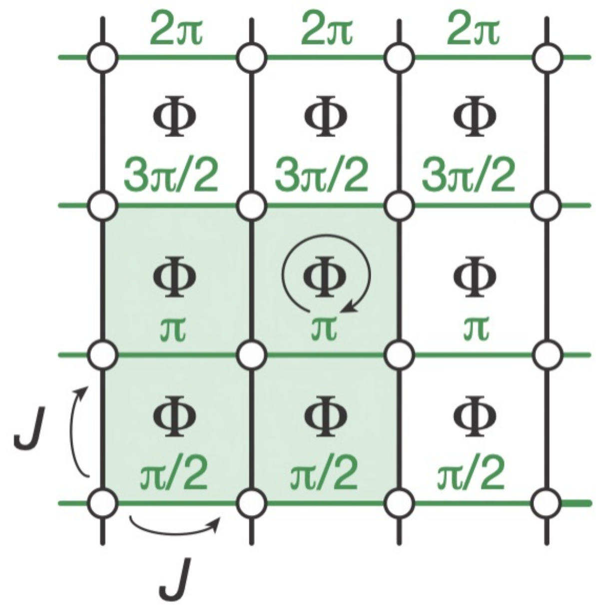
$$\hat{T}^0_y = \sum_{m,n} \hat{a}^\dagger_{m,n+1} \hat{a}_{mn}$$

$$\Rightarrow [\hat{H}(\Phi=0), \hat{T}^0_{x,y}] = 0 \; ; \; [\hat{T}^0_x, \hat{T}^0_y] = 0$$

In the presence of a vector potential (Peierls phases), however, this is no longer true!

$\Rightarrow$ The vector potential / Peierls phases $\phi^{i}_{m,n}$ are generally not invariant under discrete lattice translations, even if the $\vec{B}$-field is invariant

e.g. homogeneous flux:



$\Rightarrow$ magnetic translation operators!

(combination of translation & gauge transf.)

$$\left.\begin{aligned} \hat{T}_x^M &= \sum_{m,n} \hat{a}^\dagger_{m+1,n}\, \hat{a}_{m,n}\, e^{i\theta^x_{m,n}} \\ \hat{T}_y^M &= \sum_{m,n} \hat{a}^\dagger_{m,n+1}\, \hat{a}_{m,n}\, e^{i\theta^y_{m,n}} \end{aligned}\right\}$$

the phases $\theta^i_{m,n}$ need to be determined

<u>In general:</u> Conditions for $\theta^i_{m,n}$ can be derived using the formal requirement:

$$\boxed{[\hat{T}_i^M, \hat{H}] = 0}$$

3 <u>Homogenous magnetic fields</u>

$\rightarrow$ flux $\Phi = 2\pi\, \Phi_B / \Phi_0 = 2\pi\alpha$ per plaquette.

<u>Compute the commutator</u> $[\hat{T}_x^M, \hat{T}_y^M]$:

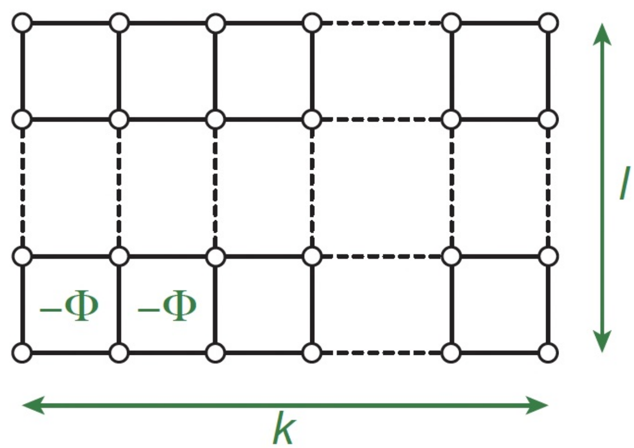
by acting, for instance, on a localized single-particle state $|i,j\rangle$.

$$\Rightarrow \boxed{e^{-i\Phi}\, \hat{T}_x^M \hat{T}_y^M = \hat{T}_y^M \hat{T}_x^M}$$

⇒ The commutator vanishes, if and only if Φ is an integer multiple of 2π

⇒ such a flux configuration is gauge-equivalent to the trivial case of zero flux.

⇒ By constructing a supercell of dimension $k \times l$, one can construct magnetic translation operators that commute with the Hamiltonian and with each other



⇒ For rational values $\alpha = p/q$ $(p, q \in \mathbb{Z})$ the commutator vanishes, if

$$\boxed{kl\,\Phi = 2\pi p \frac{kl}{q} \stackrel{!}{=} 2\pi \times \nu}$$ where $\nu \in \mathbb{Z}$

The smallest possible super cell for which

$[(\hat{T}_x^M)^k, (\hat{T}_y^M)^l] = 0$ is given by $kl = q$

and is called <u>magnetic unit cell</u>.

The area of the magnetic unit cell is q times larger than the normal lattice unit cell and contains q non-equivalent sites within the unit cell.

Using the new magnetic translation operators

$$\hat{M}_x^k \equiv (\hat{T}_x^M)^k \quad ; \quad \hat{M}_y^l = (\hat{T}_y^M)^l$$

we can use Bloch's theorem to find the eigenstates.

$$\boxed{\begin{aligned} \hat{M}_x^k |\psi_q(m,n)\rangle &= e^{iq_x ka} |\psi_q(m,n)\rangle \\ \hat{M}_y^l |\psi_q(m,n)\rangle &= e^{iq_y la} |\psi_q(m,n)\rangle \end{aligned}}$$

where a is the lattice constant and $\vec{q} = (q_x, q_y)$

is defined within the first magnetic Brillouin zone

$$-\pi/ka \leq q_x \leq \pi/ka \quad ; \quad -\pi/\ell a \leq q_y \leq \pi/\ell a$$

4 Harper – Hofstadter model

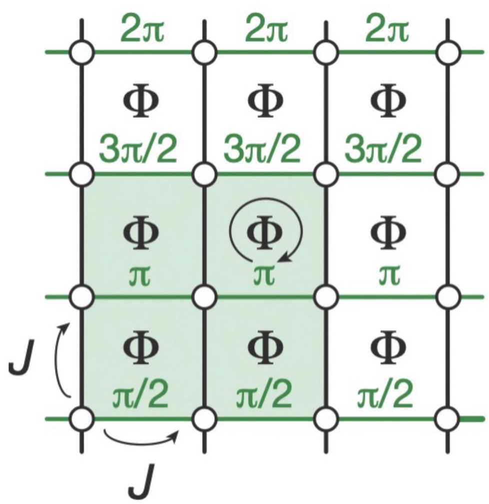
$$\boxed{\hat{H} = -J \sum_{m,n} \left(e^{-i\Phi n} \hat{a}^{\dagger}_{m+1,n} \hat{a}_{m,n} + \hat{a}^{\dagger}_{m,n+1} \hat{a}_{m,n} + h.c. \right)}$$

This Hamiltonian is expressed in the Landau gauge

→ tunneling along x is complex

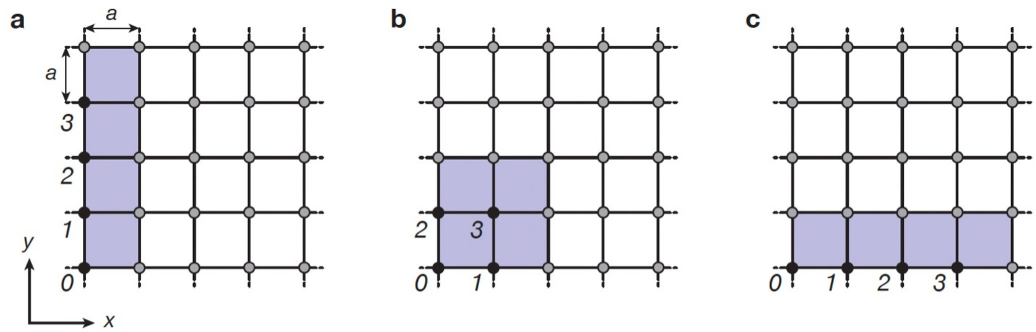
→ tunneling along y is real

Example: $\alpha = \frac{1}{4}$



Q What is the size of the unit cell?

Q Is it unique?



Compute single-particle energy spectrum for arbitrary $\alpha = p/q$

Landau gauge:

Magnetic translation operators can be chosen to have particularly simple form:

$$\hat{M}_{\hat{x}} = \sum_{m,n} \hat{a}^{\dagger}_{m+1,n} \, \hat{a}_{m,n}$$

$$\hat{M}^{q}_{y} = \sum_{m,n} \hat{a}^{\dagger}_{m,n+q} \, \hat{a}_{mn}$$

$\Rightarrow$ Take the form of simple lattice translation operators:

- translation by one lattice site along x
- translation by q lattice sites along y

$\Rightarrow$ magnetic unit cell oriented along y with dimensions $(1 \times q) \cdot a^2$

$\Rightarrow$ Area of magnetic unit cell : $\underline{\underline{A = q \cdot a^2}}$

$\Rightarrow$ The magnetic unit cell contains a flux $\underline{\underline{p \times 2\pi}}$

Ansatz for wave function:

$$\boxed{|\psi_q\rangle = \sum_{m,n} e^{iq_x m a} e^{iq_y n a} \psi_n |m,n\rangle, \quad \psi_{n+q} = \psi_n}$$

$\Rightarrow$ q non-equivalent lattice sites with amplitudes ψ_n

Inset this ansatz into Schrödinger equation:

$$E_q \psi_n = -J \left[2\cos(q_x - \Phi n)\psi_n + \right.$$
$$\left. + e^{iq_y a} \psi_{n+1} + e^{-iq_y a} \psi_{n-1} \right]$$

=> q-dimensional eigenvalue equation

$$E_{\vec{q}} \begin{pmatrix} \psi_0 \\ \vdots \\ \psi_n \end{pmatrix} = H(\vec{q}) \begin{pmatrix} \psi_0 \\ \vdots \\ \psi_n \end{pmatrix}$$

with $H(\vec{q})$ the $q \times q$ matrix

$$H(\vec{q}) = -J \begin{pmatrix} h_0 & e^{iq_y a} & 0 & & e^{-iq_y a} \\ e^{-iq_y a} & h_1 & e^{iq_y a} & & \vdots \\ 0 & e^{-iq_y a} & \ddots & & \\ \vdots & & & & 0 \\ e^{iq_y a} & & & & h_{q-1} \end{pmatrix}$$

with $h_q = 2\cos(q_x a - q \cdot \Phi)$

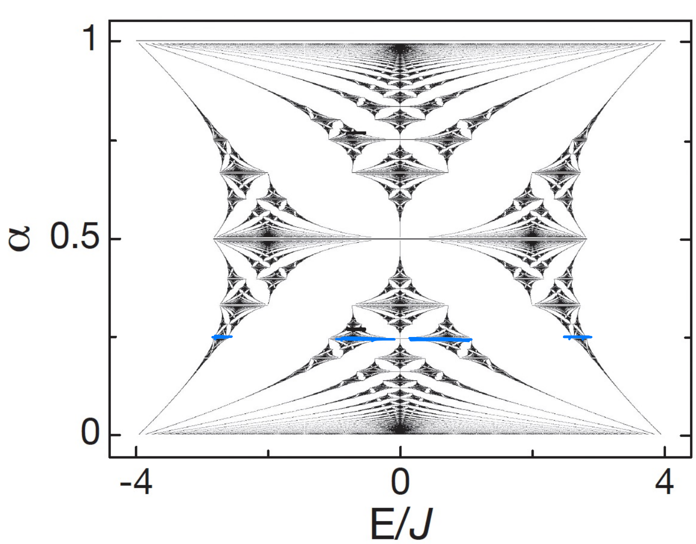
$\Rightarrow$ <u>For $\alpha \in \mathbb{Z}$:</u>

we obtain a single energy band

$$E_q = -2J\cos(q_x a) - 2J\cos(q_y a)$$

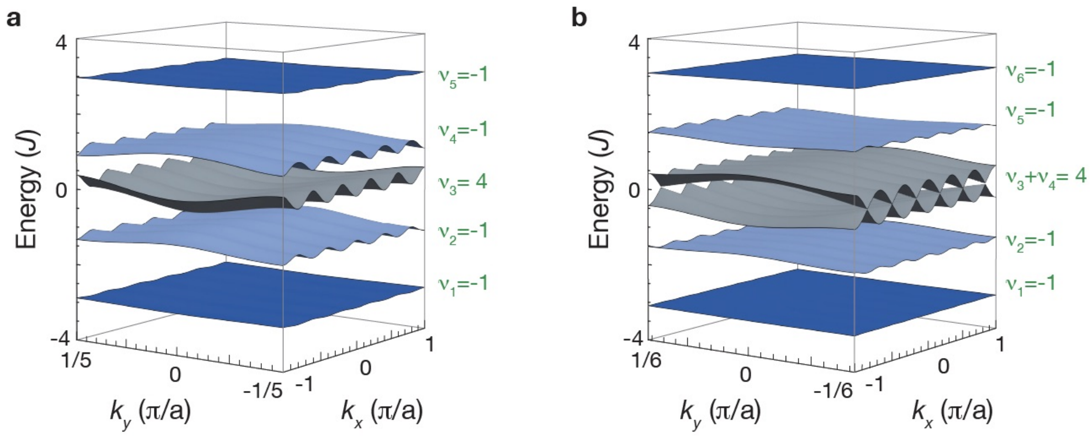
$\Rightarrow$ <u>For $\alpha = p/q$:</u>

Hofstadter butterfly



example:
$\alpha = 1/4$

Examples:



$\alpha = 1/5$ $\qquad$ $\alpha = 1/6$

In general:
- Spectrum symmetric around $E = 0$
- $\sum_i \nu_i = 0$