The Hofstadter model



One-orbital, spinless, nearest neighbor tight-binding model on a square lattice with p.b.c.

$$\boldsymbol{H} = -\sum_{\vec{r}} t \, \boldsymbol{c}_{\vec{r}+\vec{e_x}}^{\dagger} \, \boldsymbol{c}_{\vec{r}} + t \, \boldsymbol{c}_{\vec{r}+\vec{e_y}}^{\dagger} \, \boldsymbol{c}_{\vec{r}} + \text{h.c.} + \begin{array}{c} \text{magnetic} \\ \text{field term} \end{array}$$

Without a magnetic field

Bloch theorem \Rightarrow Diagonal hamiltonian in reciprocal space with

$$ilde{m{c}}_{ec{k}} := rac{1}{\sqrt{N_x \, N_y}} \sum_{ec{r}} \, \mathrm{e}^{\mathrm{i}ec{k}\cdotec{r}} \, m{c}_{ec{r}}$$



Including the magnetic field : **Peierls substitution** 3/21

How to take into account \vec{B} ? Semi-classical argument in path integral formalism

Transition amplitude :
$$\langle \vec{r}', t' | \vec{r}, t \rangle = \int_{\vec{r}(t)=\vec{r}}^{\vec{r}(t')=\vec{r}'} \mathcal{D}[\vec{r}(t)] e^{\frac{i}{\hbar}S[\vec{r}(t)]}, \quad S[\vec{r}(t)] = \int_{t}^{t'} dt \, \mathcal{L}(\vec{r}, \dot{\vec{r}})$$

Including the magnetic field : **Peierls substitution** 3/21

charge (possibly < 0)

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Including \vec{B} in the lagrangian : $\mathcal{L} = \mathcal{L}^{(0)} + e \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} \cdot \vec{A}$

$$S = S^{(0)} + e \int_{t}^{t'} \mathrm{d}t \, \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} \cdot \vec{A}(\vec{r}(t))$$
$$= S^{(0)} + e \int_{\vec{r} \to \vec{r}'} \mathrm{d}\vec{r} \cdot \vec{A}(\vec{r})$$

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Thus,

$$\langle \vec{r}', t' | \vec{r}, t \rangle \simeq \exp\left(i\frac{e}{\hbar} \int_{\vec{r} \to \vec{r}'} d\vec{r} \cdot \vec{A}(\vec{r})\right) \cdot \int_{\vec{r}}^{\vec{r}'} \mathcal{D}[\vec{r}(t)] e^{\frac{i}{\hbar} S_0[\vec{r}(t)]}$$

Including the magnetic field : **Peierls substitution** 4/21

Including the magnetic field : **Peierls substitution**

4/21



Including the magnetic field : **Peierls substitution**

4/21

- Full proof : go back to Wannier functions
- Actually "just" the consequence of enforcing U(1) gauge symmetry in $oldsymbol{H}$

Including the magnetic field : **Peierls substitution** 5/21

Warning, the Peierls path is not always the spatially shortest path (arXiv:2006.13938) :



Hofstadter hamiltonian in Landau gauge

Landau gauge $\vec{A} = \begin{bmatrix} 0 & Bx & 0 \end{bmatrix}$ and periodic boundary conditions :

- hopping $\vec{r} \to \vec{r} + \vec{e}_x$: $\int \vec{A} \cdot d\vec{r} = B \int_x^{x+a} x \, \vec{e_y} \cdot \vec{e_x} \, dx = 0$
- hopping $\vec{r} \to \vec{r} + \vec{e}_y$: $\int \vec{A} \cdot d\vec{r} = B \int_y^{y+a} x \, \vec{e_y} \cdot \vec{e_y} \, dy = B \, a \, x$ so that

$$\mathrm{e}^{\mathrm{i}\frac{e}{\hbar}\int\vec{A}\cdot\mathrm{d}\vec{r}}\boldsymbol{c}_{\vec{r}+\vec{e}_{y}}^{\dagger}\boldsymbol{c}_{\vec{r}} = \mathrm{e}^{\mathrm{i}\frac{eBax}{\hbar}}\boldsymbol{c}_{\vec{r}+\vec{e}_{y}}^{\dagger}\boldsymbol{c}_{\vec{r}} = \mathrm{e}^{2\pi\mathrm{i}n_{\phi}\frac{x}{a}}\boldsymbol{c}_{\vec{r}+\vec{e}_{y}}^{\dagger}\boldsymbol{c}_{\vec{r}} \quad \text{with} \quad n_{\phi} = \frac{eBa^{2}}{h} = \frac{e}{h}\Phi_{\mathrm{u.cell}}$$

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$$e^{i\frac{e}{\hbar}\int \vec{A} \cdot d\vec{r}} \boldsymbol{c}_{\vec{r}+\vec{e}_y}^{\dagger} \boldsymbol{c}_{\vec{r}} = e^{i\frac{eBax}{\hbar}} \boldsymbol{c}_{\vec{r}+\vec{e}_y}^{\dagger} \boldsymbol{c}_{\vec{r}} = e^{2\pi i n_{\phi}\frac{x}{a}} \boldsymbol{c}_{\vec{r}+\vec{e}_y}^{\dagger} \boldsymbol{c}_{\vec{r}} \text{ with } n_{\phi} = \frac{eBa^2}{h} = \frac{e}{h} \Phi_{\text{u.cell}}$$

$$\boldsymbol{H} = -\sum_{\vec{r}} t \, \boldsymbol{c}_{\vec{r}+\vec{e}_x}^{\dagger} \, \boldsymbol{c}_{\vec{r}} + t \, \mathrm{e}^{2\pi \mathrm{i} n_{\phi} x} \, \boldsymbol{c}_{\vec{r}+\vec{e}_y}^{\dagger} \, \boldsymbol{c}_{\vec{r}} + \mathrm{h.c.}$$

with a = 1, i.e. $x \in \mathbb{N}$.

Some symmetries

$$\boldsymbol{H} = -\sum_{\vec{r}} t \, \boldsymbol{c}_{\vec{r}+\vec{e}_x}^{\dagger} \, \boldsymbol{c}_{\vec{r}} + t \, \mathrm{e}^{2\pi \mathrm{i} n_{\phi} x} \, \boldsymbol{c}_{\vec{r}+\vec{e}_y}^{\dagger} \, \boldsymbol{c}_{\vec{r}} + \mathrm{h.c.}$$

We have $\mathrm{e}^{2\pi\mathrm{i}x}\!=\!1$, so

- transformation $n_{\phi} \rightarrow n_{\phi} + 1$: H remains invariant \Rightarrow we can restrict to $n_{\phi} \in [0, 1]$
- transformation $n_{\phi} \rightarrow 1 n_{\phi}$: $H = -\sum_{\vec{r}} t c_{\vec{r}+\vec{e}_x}^{\dagger} c_{\vec{r}} + t e^{-2\pi i n_{\phi} x} c_{\vec{r}+\vec{e}_y}^{\dagger} c_{\vec{r}} + h.c.$ which does not change eigen-energies \Rightarrow "reflection" symmetry



$$n_{\phi} = p / q$$

$$\boldsymbol{H} = -\sum_{\vec{r}} t \, \boldsymbol{c}_{\vec{r}+\vec{e}_x}^{\dagger} \, \boldsymbol{c}_{\vec{r}} + t \, \mathrm{e}^{2\pi \mathrm{i} n_{\phi} x} \, \boldsymbol{c}_{\vec{r}+\vec{e}_y}^{\dagger} \, \boldsymbol{c}_{\vec{r}} + \mathrm{h.c.}$$

Periodic boundary conditions along \boldsymbol{x} impose that

$$e^{2\pi i n_{\phi} x}|_{x=N_x} = e^{2\pi i n_{\phi} x}|_{x=0}$$

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i.e.

$$n_{\phi} N_x \in \mathbb{N} \quad \Rightarrow \quad \left[n_{\phi} = \frac{n}{N_x}, \ n \in \mathbb{N} \right]$$

Thus $n_{\phi} = \frac{p}{q} \in \mathbb{Q}$. We can always choose p, q coprime.

Flux is quantized in p.b.c. because we are on a closed surface (\sim magnetic monopole).

$$\boldsymbol{H} = -\sum_{x,y} t \left(\boldsymbol{c}_{x+1,y}^{\dagger} \boldsymbol{c}_{x,y} + e^{2\pi i n_{\phi} x} \boldsymbol{c}_{x,y+1}^{\dagger} \boldsymbol{c}_{x,y} + h.c. \right)$$

Still y-translation invariant. But the phase breaks the x-translation invariance...

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However, we can thus partially diagonalize the hamiltonian by going in Fourier space $y \rightarrow \tilde{k}_y$ Mixed annihilation operator :

$$ilde{oldsymbol{c}}_{x,\mathtt{k}_y} := rac{1}{\sqrt{N_y}} \sum_y \, \mathrm{e}^{2\pi\mathrm{i}rac{\mathtt{k}_y y}{N_y}} oldsymbol{c}_{x,y} \quad ext{where} \quad \mathtt{k}_y \!\in \! [\![0,N_y]\!]$$

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We compute

$$\sum_{\mathbf{k}_{y}} e^{2\pi i \frac{\mathbf{k}_{y}}{N_{y}}n} \tilde{\boldsymbol{c}}_{x,\mathbf{k}_{y}}^{\dagger} \tilde{\boldsymbol{c}}_{x',\mathbf{k}_{y}} = \frac{1}{N_{y}} \sum_{y,y'} \sum_{\mathbf{k}_{y}} e^{2\pi i \frac{\mathbf{k}_{y}}{N_{y}}(-y+y'+n)} \tilde{\boldsymbol{c}}_{x,y}^{\dagger} \tilde{\boldsymbol{c}}_{x',y'} = \sum_{y} \tilde{\boldsymbol{c}}_{x,y+n}^{\dagger} \tilde{\boldsymbol{c}}_{x',y}$$

$$\boldsymbol{H} = -\sum_{x,y} t \left(\boldsymbol{c}_{x+1,y}^{\dagger} \boldsymbol{c}_{x,y} + e^{2\pi i n_{\phi} x} \boldsymbol{c}_{x,y+1}^{\dagger} \boldsymbol{c}_{x,y} + h.c. \right)$$

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SO

$$\boldsymbol{H} = -\sum_{x,\mathbf{k}_y} t\left(\tilde{\boldsymbol{c}}_{x+1,\mathbf{k}_y}^{\dagger} \tilde{\boldsymbol{c}}_{x,\mathbf{k}_y} + e^{2\pi i (n_{\phi}x + \mathbf{k}_y/N_y)} \tilde{\boldsymbol{c}}_{x,\mathbf{k}_y}^{\dagger} \tilde{\boldsymbol{c}}_{x,\mathbf{k}_y} + \text{h.c.}\right)$$

It is ky-diagonal !

$$\begin{aligned} \boldsymbol{H} &= -\sum_{x,\mathbf{k}_{y}} t\left(\tilde{\boldsymbol{c}}_{x+1,\mathbf{k}_{y}}^{\dagger} \tilde{\boldsymbol{c}}_{x,\mathbf{k}_{y}} + e^{2\pi i (n_{\phi}x+\mathbf{k}_{y}/N_{y})} \tilde{\boldsymbol{c}}_{x,\mathbf{k}_{y}}^{\dagger} \tilde{\boldsymbol{c}}_{x,\mathbf{k}_{y}} + \text{h.c.}\right) \\ &= -\sum_{x,\mathbf{k}_{y}} t\left(\tilde{\boldsymbol{c}}_{x+1,\mathbf{k}_{y}}^{\dagger} \tilde{\boldsymbol{c}}_{x,\mathbf{k}_{y}} + \tilde{\boldsymbol{c}}_{x,\mathbf{k}_{y}}^{\dagger} \tilde{\boldsymbol{c}}_{x+1,\mathbf{k}_{y}} + 2t \cos\left(2\pi n_{\phi}x+\mathbf{k}_{y}\frac{2\pi}{N_{y}}\right) \tilde{\boldsymbol{c}}_{x,\mathbf{k}_{y}}^{\dagger} \tilde{\boldsymbol{c}}_{x,\mathbf{k}_{y}}\right) \\ &= \sum_{\mathbf{k}_{y}} \boldsymbol{H}'(\mathbf{k}_{y}) \end{aligned}$$

with

$$\boldsymbol{H}'(\mathbf{k}_y) = -t \sum_x \, \tilde{\boldsymbol{c}}_{x+1}^{\dagger} \, \tilde{\boldsymbol{c}}_x \, + \, \tilde{\boldsymbol{c}}_x^{\dagger} \, \tilde{\boldsymbol{c}}_{x+1} + 2 \cos \! \left(2\pi \, n_\phi \, x + \mathbf{k}_y \, \frac{2\pi}{N_y} \right) \tilde{\boldsymbol{c}}_x^{\dagger} \, \tilde{\boldsymbol{c}}_x$$

Note : at first sight, k_y looks like an irrelevant phase (with p.b.c.), but it is not exactly.

Hofstadter butterfly



At B = 0, at the bottom of the band, the electron has an effective mass $m^* = \frac{\hbar^2}{t a^2}$. At $B \neq 0$ such that $\ell_B = \sqrt{\hbar/e B} \ll a$:



 \Rightarrow negligible lattice effects \Rightarrow Landau levels

$$E_n \simeq \hbar \, \omega_c \left(n + \frac{1}{2} \right)$$
 with $\omega_c = \frac{e \, B}{m^*}$

Indeed, we observe a fan of Landau levels :



$$E_n \simeq \hbar \,\omega_c \left(n + \frac{1}{2}\right)$$
 with $\omega_c \propto n_\phi$

Justification :

$$\boldsymbol{H}'(\mathbf{k}_y) = -t \sum_x \, \tilde{\boldsymbol{c}}_{x+a}^{\dagger} \, \tilde{\boldsymbol{c}}_x + \, \tilde{\boldsymbol{c}}_x^{\dagger} \, \tilde{\boldsymbol{c}}_{x+a} + 2\cos\left(2\pi \, n_\phi \frac{x}{a} + \mathbf{k}_y \frac{2\pi \, a}{N_y}\right) \tilde{\boldsymbol{c}}_x^{\dagger} \, \tilde{\boldsymbol{c}}_x$$

Let \boldsymbol{H} on a wavefunction $\psi(\boldsymbol{x},\boldsymbol{y})$:

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Let H on a wavefunction $\psi(x, y)$: y-part is a Bloch wave, and $H'(k_y)$ acts on the x-part :

$$E\psi_{\mathbf{k}_{y}}(x) = \mathbf{H}'(\mathbf{k}_{y})\psi_{\mathbf{k}_{y}}(x) = -t\left(e^{-a\partial_{x}} + e^{+a\partial_{x}} + 2\cos\left(2\pi n_{\phi}\frac{x}{a} + \mathbf{k}_{y}\frac{2\pi a}{N_{y}}\right)\right)\psi_{\mathbf{k}_{y}}(x)$$

(indeed,
$$\tilde{\boldsymbol{c}}_{x+a}^{\dagger} \tilde{\boldsymbol{c}}_{x} = (\boldsymbol{c}_{x,y}^{\dagger} + a \,\partial_x \, \boldsymbol{c}_{x,y}^{\dagger} + \cdots) \, \boldsymbol{c}_{x,y} = (e^{a\partial_x} \, \boldsymbol{c}_{x,y}^{\dagger}) \, \boldsymbol{c}_{x,y}).$$

This is Harper's equation.

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Continuum limit $a \ll \ell_B \iff e B \ll \hbar/a^2$:

 $\psi_{\mathbf{k}_y}(x)$ varies slowly (envelope function) and the \cos can be expanded :

$$E \psi_{\mathbf{k}_{y}}(x) \simeq -t \left(2 + a^{2} \partial_{x}^{2} + 2 - \left(\mathbf{k}_{y} \frac{2\pi a}{N_{y}} + 2\pi n_{\phi} \frac{x}{a} \right)^{2} \right) \psi_{\mathbf{k}_{y}}(x)$$

$$\left[m^{*} = \frac{2 \hbar^{2}}{t a^{2}}, n_{\phi} = \frac{e B a^{2}}{h} \right] = -\left(\operatorname{cst} - \frac{t a^{2}}{\hbar^{2}} \frac{(-i \hbar \partial_{x})^{2}}{2} - \frac{t a^{2}}{\hbar^{2}} \left(\frac{2\pi \hbar \mathbf{k}_{y}}{N_{y}} + e B x \right)^{2} \right) \psi_{\mathbf{k}_{y}}(x)$$

$$= \frac{1}{2 m^{*}} \left(\operatorname{cst} + p_{x}^{2} + (p_{y}^{2} + e B x)^{2} \right) \psi_{\mathbf{k}_{y}}(x)$$

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$$= \frac{1}{2 m^{*}} \left(\operatorname{cst} + \mathbf{p}_{x}^{2} + (\mathbf{p}_{y}^{2} + e B \mathbf{x})^{2} \right) \psi_{\mathbf{k}_{y}}(x)$$

This is the Landau hamiltonian !

$$\boldsymbol{H}_{L} = \frac{1}{2\,m^{*}} \left(\boldsymbol{p}_{x}^{2} + (\boldsymbol{p}_{y}^{2} + e\,B\,\boldsymbol{x})^{2} \right)$$

Are we bound to always be $n_{\phi} \ll 1$?

Cf. lecture :

$$\ell_B = \frac{26 \,\mathrm{nm}}{\sqrt{B\left[T\right]}} \gg \quad a = \begin{cases} 0.142 \,\mathrm{nm} & \text{for graphene} \\ 0.565 \,\mathrm{nm} & \text{for GaAs} \end{cases}$$
$$\Leftrightarrow \qquad B \qquad \gg \qquad \begin{cases} 3 \cdot 10^4 \,T & \text{for graphene} \\ 2 \cdot 10^3 \,T & \text{for GaAs} \end{cases}$$

- In HbN substrate with Moire superlattice, high field (\sim 40 T) \Rightarrow 0-energy Landau level \Rightarrow massless Dirac fermions;
- While in graphene, 0 Landau level split into 2 non-0 energy levels.



Particle-hole symmetry

How to explain the $E \leftrightarrow -E$ symmetry ? Consider the transformation $\Gamma: \mathbf{c}_{x,y} \mapsto (-1)^{x+y} \mathbf{c}_{x,y}$. $\mathbf{H} = -t \sum_{x,y} \mathbf{c}_{x+1,y}^{\dagger} \mathbf{c}_{x,y} + e^{2\pi i n_{\phi} x} \mathbf{c}_{x,y+1}^{\dagger} \mathbf{c}_{x,y} + h.c.$ $\mapsto -t \sum_{x,y} (-1)^{2x+1+2y} \mathbf{c}_{x+1,y}^{\dagger} \mathbf{c}_{x,y} + (-1)^{2x+2y+1} e^{2\pi i n_{\phi} x} \mathbf{c}_{x,y+1}^{\dagger} \mathbf{c}_{x,y} + h.c.$

$$\mapsto -t \sum_{\vec{r}} \underbrace{(-1)^{2x+1+2y}}_{=-1} c_{x+1,y}^{\dagger} c_{x,y} + \underbrace{(-1)^{2x+2y+1}}_{=-1} e^{2\pi i n_{\phi} x} c_{x,y+1}^{\dagger} c_{x,y} + \text{h.c.}$$
$$= -H \quad \Rightarrow \quad \boxed{\Gamma H \Gamma^{-1} = -H}$$

Consequence : if $\psi(x, y)$ is an eigenstate of energy E, then $(-1)^{x+y}\psi(x, y)$ is a *different* state of energy $-E \Rightarrow$ spectrum is symmetric around 0.

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This is because a square lattice is bipartite. A triangular lattice would not have this symmetry :



Open boundary conditions

$$N_x = 120; N_y = 60; n_\phi = \frac{1}{3}$$



The x-translation invariance is broken... and a $N_x \times N_x$ hamiltonian is slow to diagonalize.

The x-translation invariance is broken... and a $N_x \times N_x$ hamiltonian is slow to diagonalize. But...

$$\boldsymbol{H} = -\sum_{x,y} t \left(\boldsymbol{c}_{x+1,y}^{\dagger} \boldsymbol{c}_{x,y} + e^{2\pi i n_{\phi} x} \boldsymbol{c}_{x,y+1}^{\dagger} \boldsymbol{c}_{x,y} + h.c. \right)$$

is still invariant when we translate along x by q sites $(n_{\phi} = {}^{p}\!/_{q})$:

$$e^{2\pi i n_{\phi} x} c_{x,y+1}^{\dagger} c_{x,y} \quad \mapsto \underbrace{e^{2\pi i n_{\phi}(x+q)}}_{= e^{2\pi i p \frac{x+q}{q}}} c_{x+q,y+1}^{\dagger} c_{x+q,y}$$
$$= e^{2\pi i p \frac{x}{q}}$$
$$= e^{2\pi i p \frac{x}{q}} = e^{2\pi i n_{\phi} x}$$

+ p.b.c.





Bloch hamiltonian with unit cell $q \times 1$ (with p flux quanta) \Rightarrow BZ q-folded

[play with the code, looking at the spectrum for various small fields]



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$$\boldsymbol{H}'(\mathbf{k}_y) = -t \sum_x \, \tilde{\boldsymbol{c}}_{x+1}^{\dagger} \, \tilde{\boldsymbol{c}}_x + \, \tilde{\boldsymbol{c}}_x^{\dagger} \, \tilde{\boldsymbol{c}}_{x+1} + 2\cos(2\pi \, n_\phi \, x + k_y) \, \tilde{\boldsymbol{c}}_x^{\dagger} \, \tilde{\boldsymbol{c}}_x \quad \left(k_y = \mathbf{k}_y \, \frac{2\pi}{N_y}\right)$$

$$\sum_{x} \cos(2\pi n_{\phi} x) \dots = \sum_{j} \cos(2\pi n_{\phi} j) \sum_{n} \dots j \in \llbracket 1, q \rrbracket \quad x = n q + j$$

Introduce

$$\tilde{\tilde{c}}_{j,k_x,k_y} := \frac{1}{\sqrt{q}} \sum_{n} e^{2\pi i k_x n} \tilde{c}_{nq+j,k_y}, \quad \tilde{\tilde{c}}_{q,k_x,k_y} \equiv \tilde{\tilde{c}}_{0,k_x,k_y}$$

$$\boldsymbol{H}'(k_y) = -t \sum_{k_x} \boldsymbol{H}''(k_x, k_y)$$

with

$$\boldsymbol{H}'' = \sum_{j} e^{-2\pi i k_x} \tilde{\tilde{c}}_{j+1,k_x}^{\dagger} \tilde{\tilde{c}}_{j,k_x} + e^{2\pi i k_x} \tilde{\tilde{c}}_{j,k_x}^{\dagger} \tilde{\tilde{c}}_{j+1,k_x} + 2\cos(2\pi n_\phi j + k_y) \tilde{\tilde{c}}_{j,k_x}^{\dagger} \tilde{\tilde{c}}_{j,k_x}$$