URG Analysis of Electron in a Periodic Potential

Role of the center of mass

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The Big Picture

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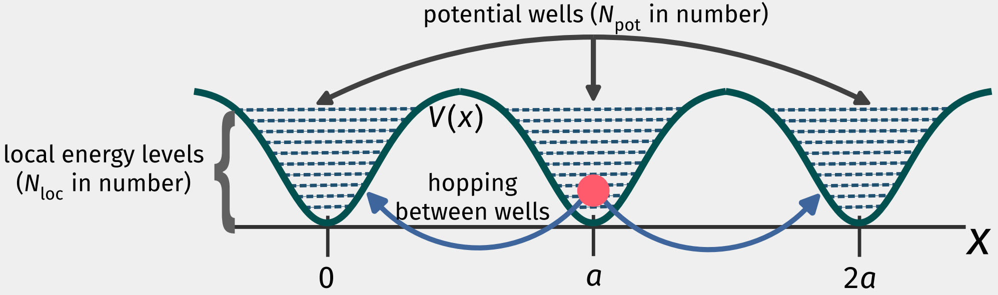
- We conclude by connecting this problem to that of the **IQHE**.

The Problem of a Particle in a Periodic Potential (PPP)

$$H = \int_{-\infty}^{\infty} \mathrm{d}x \, c^\dagger(x) \left[\hat{p}^2 / 2m + V(x) \right] c(x), \quad V(x + a) = V(x)$$



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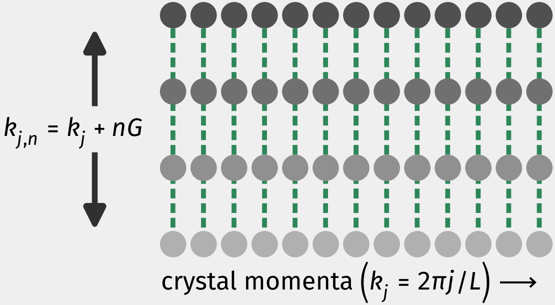
Potential only connects momentum states separated by a reciprocal lattice vector.

$$\langle k + q | V | k \rangle = \delta_{q,G} V(G)$$

Leads to conserved **crystal momenta**: $\left\{ k_j < G \right\}$



The PPP as a Particle on a Circle

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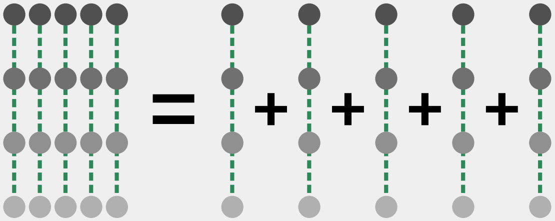
The conserved crystal momenta leads to a block-diagonal form of the Hamiltonian.

$$H = \sum_k H(k), \quad H(k) \sim \left(-i\hbar \frac{\partial}{\partial x'} + \hbar k\right)^2 + V(x')$$

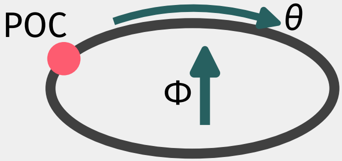


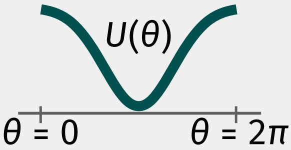
The PPP as a Particle on a Circle

Define dimensionless position and momentum.

$$H(k) = \frac{\hbar^2}{2ma^2}\left(\hat{Q} + \Phi/2\pi\right)^2 + U(\theta)$$

Hamiltonian is that of a **particle on a circle**. Flux is $\Phi = ka$.



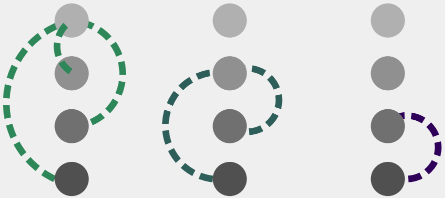


URG Analysis of the POC

URG Analysis of the PAC

Resolve fluctuations in angular momentum states by applying unitary transformations.

$$\Delta U_{ij}^{(l)}(\omega) = \frac{U_{il}U_{lj}}{\omega - \varepsilon(Q_l + \Phi/2\pi)}, \quad U_{ij} = U(Q_i - Q_j)$$



URG transformations $\longrightarrow$

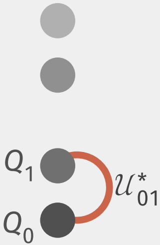
Appearance of band gaps

Effective Hamiltonian for the final two states:

$$H^*_{01} = \varepsilon^*(Q_0)\,|Q_0\rangle\langle Q_0| + \varepsilon^*(Q_1)\,|Q_1\rangle\langle Q_1| + \left(U^*_{01}\,|Q_1\rangle\langle Q_0| + \text{h.c.}\right)$$

Diagonalise the final Hamiltonian: $E_\pm = \varepsilon^* \pm |U^*_{01}|$

Gives the **shifts in energies**: $$\Delta\varepsilon^* \simeq \frac{|U^*_{01}|^2}{\varepsilon^* \pm |U^*_{01}| - \varepsilon^*} \simeq \pm|U^*_{01}|$$



Appearance of band gaps

Allow the flux Φ to vary:

$$\varepsilon^*(\Phi) - |U^*_{01}|; \Phi = ak$$

Creates the **first band**!

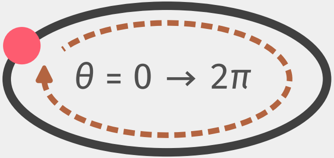
Dispersion for the lowest band

Fixed point Hamiltonian for the lowest state is of the form:

$$\varepsilon^*(Q_0)\,|Q_0\rangle\langle Q_0|$$

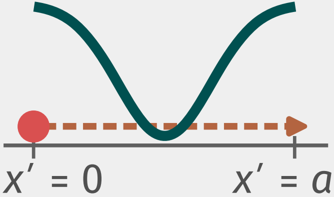
Involves only longest-range hopping:

$$\frac{1}{2}\varepsilon^*(2\pi)\left(\hat{n}(0)+\hat{n}(2\pi)\right)+\frac{1}{2}\varepsilon^*(2\pi)\left(c^\dagger(0)c(2\pi)+\text{h.c.}\right)$$



Can be transformed back to real space: $\theta \rightarrow x'$

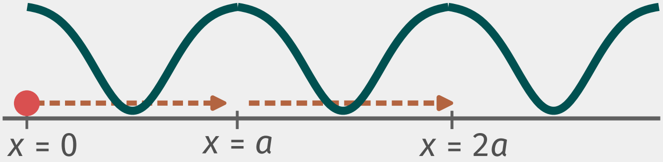
$$\frac{1}{2}\varepsilon^*(2\pi)\left(\hat{n}(0)+\hat{n}(a)\right)+\frac{1}{2}\varepsilon^*(a)\left(c^\dagger(0)c(a)+\text{h.c.}\right)$$



Dispersion for the lowest band

Reintroduce the flux.

Equivalent to translating over all lattice sites.



Leads to a tight-binding model!

$$H_{TB} = \varepsilon^*(2\pi) \sum_{j=0}^{N_{\text{well}}-1} \hat{n}(ja) + \frac{1}{2}\varepsilon^*(a) \sum_{j=0}^{N_{\text{well}}-1} \left(c^\dagger(ja)c((j+1)a) + \text{h.c.} \right)$$

Insights on the crystal momentum, role of the POC, and Bloch's theorem

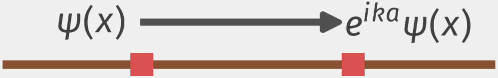
The crystal momentum as a magnetic flux

- Crystal momentum acts like a gauge field for the POC
- Leads to twisted boundary conditions for the POC
- Topological in nature (akin to a θ–term in the action)

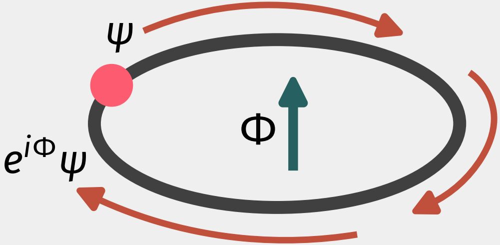
Berry phase and Bloch's theorem

Bloch's theorem for periodic potential:

$$\psi_k(x + ma) = e^{-ikam}\psi_k(x)$$



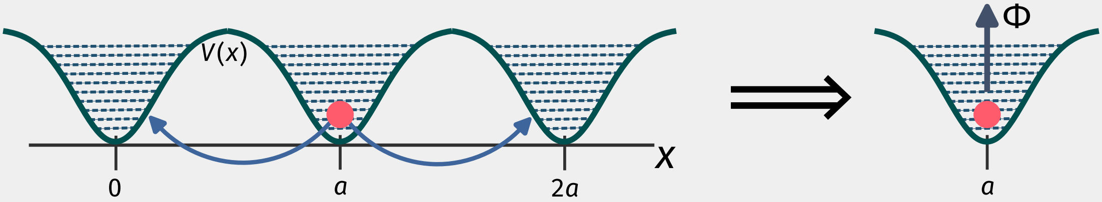
Equivalent to the Berry phase acquired in the presence of a flux!



Crystal momentum therefore acts as a Berry phase, sensitive to the topology of PBC!

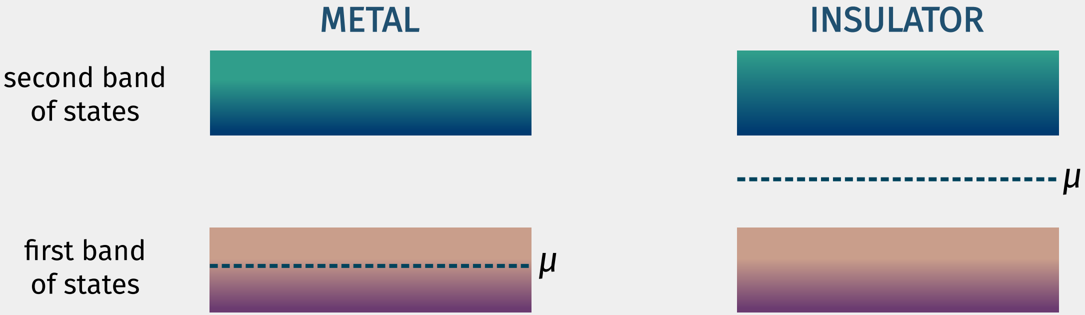
The POC as a centre of mass

The PPP problem can be mapped to the problem of a single well but in a variable flux.



The POC can be thought of as the **center of mass** degree of freedom.

METAL-INSULATOR TRANSITION UPON TUNING CHEMICAL POTENTIAL

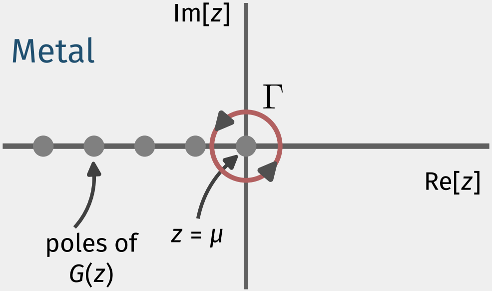


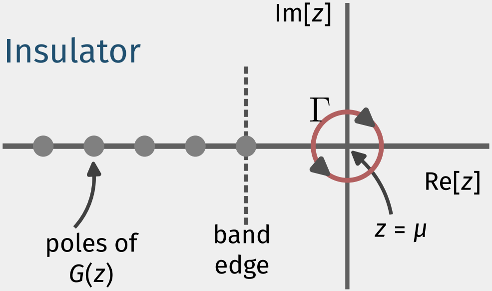
possibility of spectral flow

no possibility of spectral flow

Topological nature of the transition

Greens function has poles at the energy eigenvalues: $G(z) = \sum \left(z - E_i(\Phi_m)\right)^{-1}$





Fermi level occupancy can be detected through presence of pole:

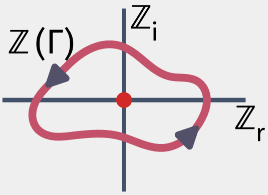
$$n_{\mathrm{FL}} = \frac{1}{2\pi i} f_{\mathrm{FD}}(\mu) \oint_{\Gamma} \mathrm{d}z\, \mathrm{Tr}\left[\mathbb{G}(z)\right]$$

Topological nature of the transition

Fermi level occupancy can be expressed as a winding number:

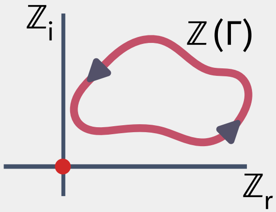
$$n_{\mathrm{FL}} = \frac{1}{2\pi i}\oint_{\Gamma} \mathrm{dz}\, \frac{d}{dz} \ln \mathrm{Det}\left[\mathrm{G}^{-1}\right] = \text{some integer}$$

Counts the number of times $\ln \mathrm{Det}\left[\mathrm{G}^{-1}\right](\Gamma)$ winds around the origin.



Metal

$$\mathbb{Z} = \ln \mathrm{Det}\left[\mathbf{G}^{-1}\right]$$



Insulator

THANK YOU.