URG Analysis of Electron in a Periodic Potential

Role of the center of mass

Abhirup Mukherjee, Siddhartha Lal

Emergent Phenomena in Quantum Matter Group
Department of Physical Sciences, IISER Kolkata

July 21, 2023

The Big Picture

- We reduce the problem to that of a **particle placed on a ring** in a periodic potential and a gauge field (generated by the crystal momenta).

The Big Picture

- We reduce the problem to that of a **particle placed on a ring** in a periodic potential and a gauge field (generated by the crystal momenta).
- By applying the URG to this problem, we show the **emergence of bands**.

The Big Picture

- We reduce the problem to that of a **particle placed on a ring** in a periodic potential and a gauge field (generated by the crystal momenta).
- By applying the URG to this problem, we show the **emergence of bands**.
- We then elucidate certain important physical ideas like the role of the particle on a circle problem as the **center of mass** of the system and the connection of the gauge field to Bloch's theorem.

The Big Picture

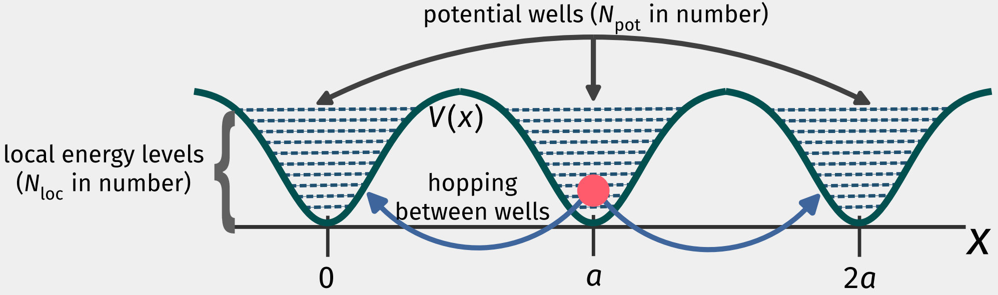
- We reduce the problem to that of a **particle placed on a ring** in a periodic potential and a gauge field (generated by the crystal momenta).
- By applying the URG to this problem, we show the **emergence of bands**.
- We then elucidate certain important physical ideas like the role of the particle on a circle problem as the **center of mass** of the system and the connection of the gauge field to Bloch's theorem.
- We demonstrate that the metal-insulator transition observed upon tuning the chemical potential occurs through the change of a **topological number**.

The Big Picture

- We reduce the problem to that of a **particle placed on a ring** in a periodic potential and a gauge field (generated by the crystal momenta).
- By applying the URG to this problem, we show the **emergence of bands**.
- We then elucidate certain important physical ideas like the role of the particle on a circle problem as the **center of mass** of the system and the connection of the gauge field to Bloch's theorem.
- We demonstrate that the metal-insulator transition observed upon tuning the chemical potential occurs through the change of a **topological number**.
- We conclude by connecting this problem to that of the **IQHE**.

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

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



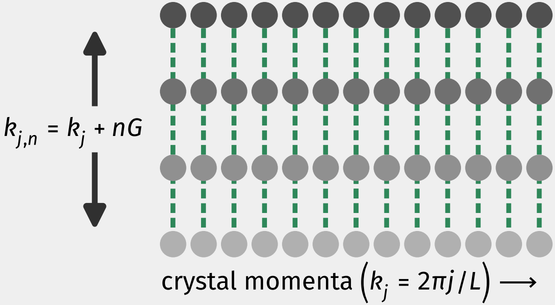
The Problem of a Particle in a Periodic Potential (PPP)

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

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**: $\left\{ k_j < G \right\}$

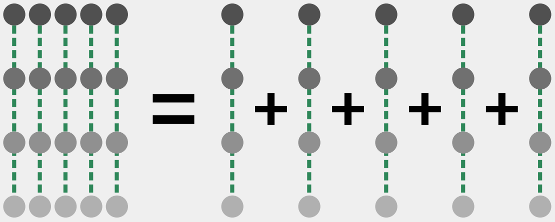


The PPP as a Particle on a Circle

The PPP as a Particle on a Circle

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

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

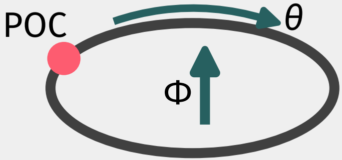


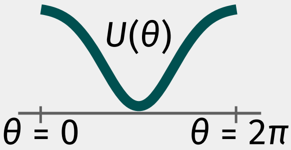
The PPP as a Particle on a Circle

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 $\Phi = ka$.



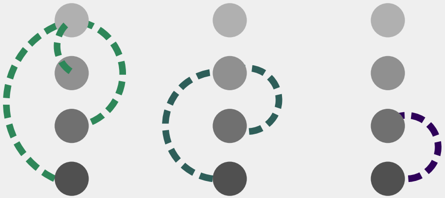


URG Analysis of the POC

URG Analysis of the POC

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 ⟶

Mukherjee 2020.

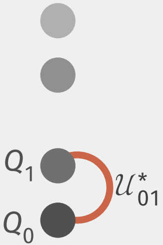
Appearance of band gaps

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**!

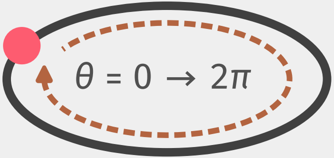
Dispersion for the lowest band

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

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

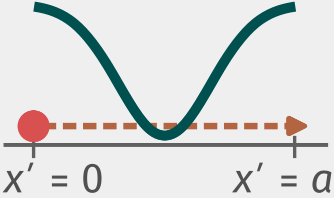
Involves only **longest-range hopping**:

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



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

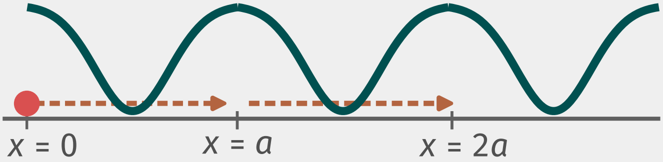
$$\frac{1}{2}\varepsilon^*(2\pi)\left(\hat{n}(0)+\hat{n}(a)\right)+\frac{1}{2}\varepsilon^*(a)\left(c^\dagger(0)c(a)+\text{h.c.}\right)$$



Dispersion for the lowest band

Reintroduce the flux.

Equivalent to translating over all lattice sites.



Leads to a **tight-binding model**!

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

Rajaraman 1982; Weigert 1994.

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

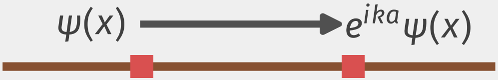
The crystal momentum as a magnetic flux

- 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)

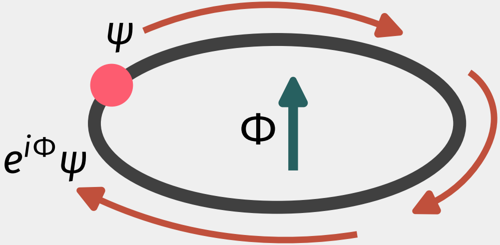
Berry phase and Bloch’s theorem

Bloch's theorem for periodic potential:

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



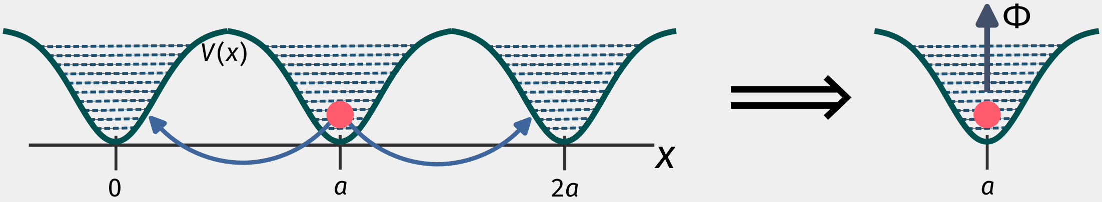
Equivalent to the **Berry phase** acquired in the presence of a flux!



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.



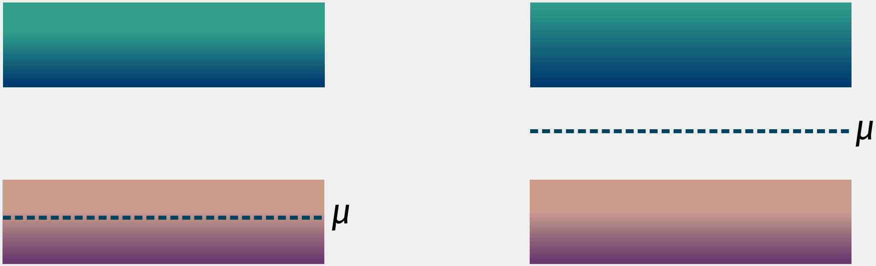
The POC can be thought of as the **center of mass** degree of freedom.

Metal-insulator transition upon tuning chemical potential

METAL | **INSULATOR**

second band of states

first band of states

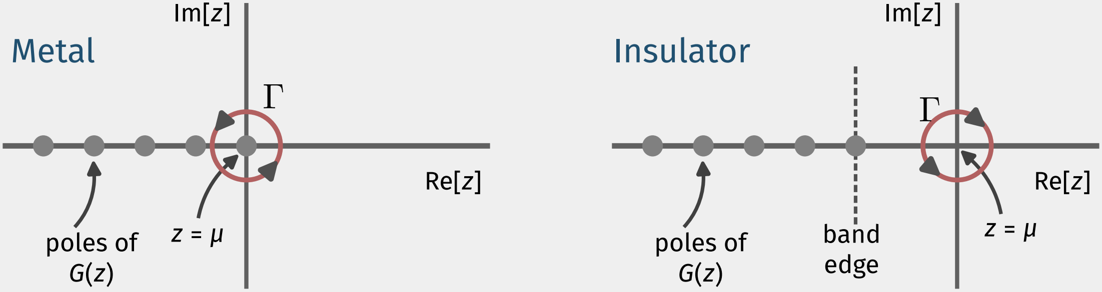


possibility of spectral flow

no possibility of spectral flow

Seki et al. 2017.

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**:

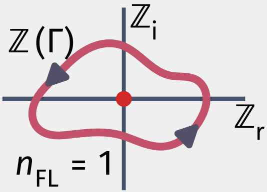
$$n_{\mathrm{FL}} = \frac{1}{2\pi i} f_{\mathrm{FD}}(\mu) \oint_{\Gamma} \mathrm{d}z\, \mathrm{Tr}\left[\mathbb{G}(z)\right]$$

Topological nature of the transition

Fermi level occupancy can be expressed as a **winding number**:

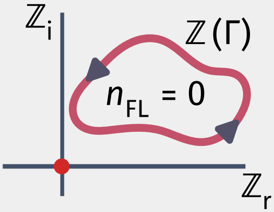
$$n_{\mathrm{FL}} = \frac{1}{2\pi i} \oint_{\Gamma} \mathrm{d}z \, \frac{d}{dz} \ln \mathrm{Det}\left[\mathrm{G}^{-1}\right] = \text{some integer}$$

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

Effect of two-particle interactions

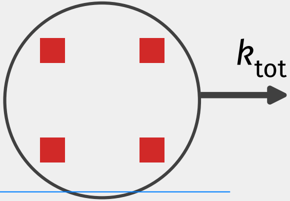
Effect of two-particle interactions

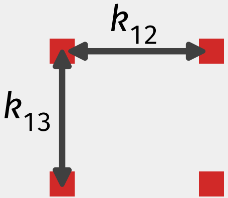
Consider multiple particles $\{i\}$ in the band in which the chem. pot. resides.

$$H = \sum_i \frac{\hbar^2}{2m} k_i^2$$

Can be **separated** into commuting total momentum and relative momentum parts:

$$H = \frac{\hbar^2}{2N_e m} k_{\text{tot}}^2 + \frac{\hbar^2}{2N_e m} \sum_{i>j} k_{ij}^2$$





Tao et al. 1986.

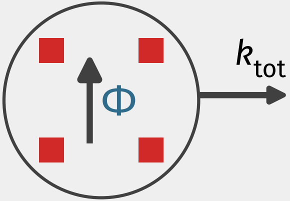
Effect of two-particle interactions

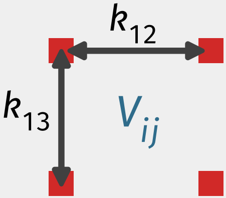
Introduce **inter-particle interaction** $V(r_i - r_j)$ and an Aharanov-Bohm flux Φ.

$$H = \frac{\hbar^2}{2N_e m}\left(k_{\mathrm{tot}} - \Phi\right)^2 + \frac{\hbar^2}{2N_e m}\sum_{i>j}\left(k_{ij}^2 + V(r_i - r_j)\right)$$

Flux couples to total part, interactions to relative part!

Interactions leave spectral flow **unaffected**!





Tao et al. 1986.

The next step: Introducing a magnetic field

The next step: Introducing a magnetic field

The next step is to perform a similar analysis in the presence of a **magnetic field**.

$$H = \int_{-\infty}^{\infty} \mathrm{d}x \, c^\dagger(x) \left[\frac{1}{2m} (\hat{p} - A(x))^2 + V(x) \right] c(x), \quad V(x+a) = V(x)$$

- Can we see the emergence of the **Landau levels** as the quantum fluctuations in $V(x)$ and $A(x)$ are resolved?
- Can we obtain a **transition** as the magnetic field is tuned?
- What is the **theory** for the Hamiltonian levels precisely at the transition?

Thouless et al. 1982.

THANK YOU

- MUKHERJEE, ANIRBAN (2020). ``Unitary renormalization group for correlated electrons''. PhD thesis. Indian Institute of Science Education and Research Kolkata.
- RAJARAMAN, R. (1982). *Solitons and Instantons: An Introduction to Solitons and Instantons in Quantum Field Theory*. North-Holland personal library. North-Holland Publishing Company. ISBN: 9780444862297.
- SEKI, KAZUHIRO AND SEIJI YUNOKI (2017). ``Topological interpretation of the Luttinger theorem''. In: *Physical Review B* 96.8, p. 085124.
- TAO, RONGJIA AND FDM HALDANE (1986). ``Impurity effect, degeneracy, and topological invariant in the quantum Hall effect''. In: *Physical Review B* 33.6, p. 3844.
- THOULESS, DJ ET AL. (1982). ``Quantized Hall conductance in a two-dimensional periodic potential''. In: *Physical Review Letters* 49.6, p. 405.
- WEIGERT, STEFAN (1994). ``Topological quenching of the tunnel splitting for a particle in a double-well potential on a planar loop''. In: *Phys. Rev. A* 50 (6), pp. 4572–4581.