



Aalto University  
School of Science

# Superfluidity and interactions in topologically and geometrically nontrivial bands

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WE-Heraeus-Seminar on “Ultracold Quantum  
Gases – Current Trends and Future Perspectives”  
Bad Honnef, Germany  
9th May 2016

# Contents

Superfluidity in topologically non-trivial flat bands

S. Peotta, PT

Nature Communications 6, 8944 (2015)

Geometric origin of superfluidity in the Lieb lattice flat band

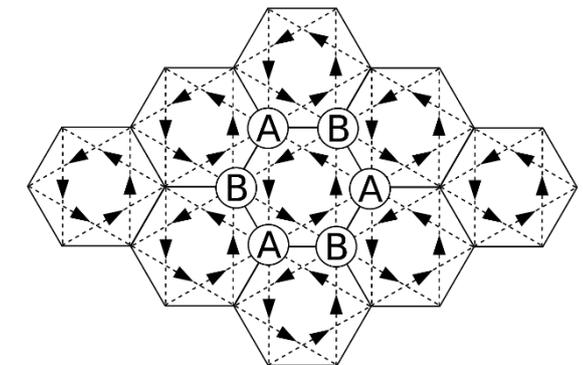
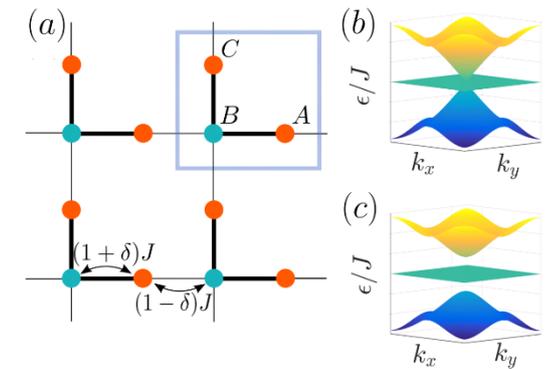
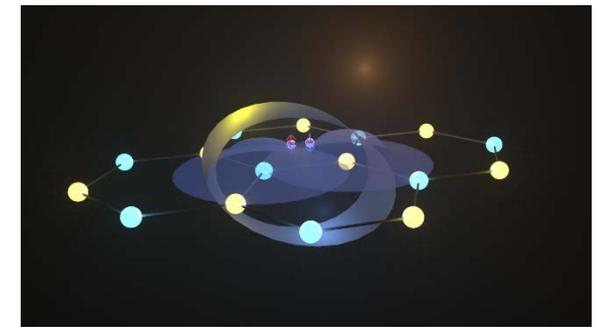
A. Julku, S. Peotta, T.I. Vanhala, D-H. Kim, PT

arXiv:1603.03237 (2016)

Topological phases in the Haldane-Hubbard model

T.I. Vanhala, T. Siro, L. Liang, M. Troyer, A. Harju, PT,

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Sebastiano Peotta

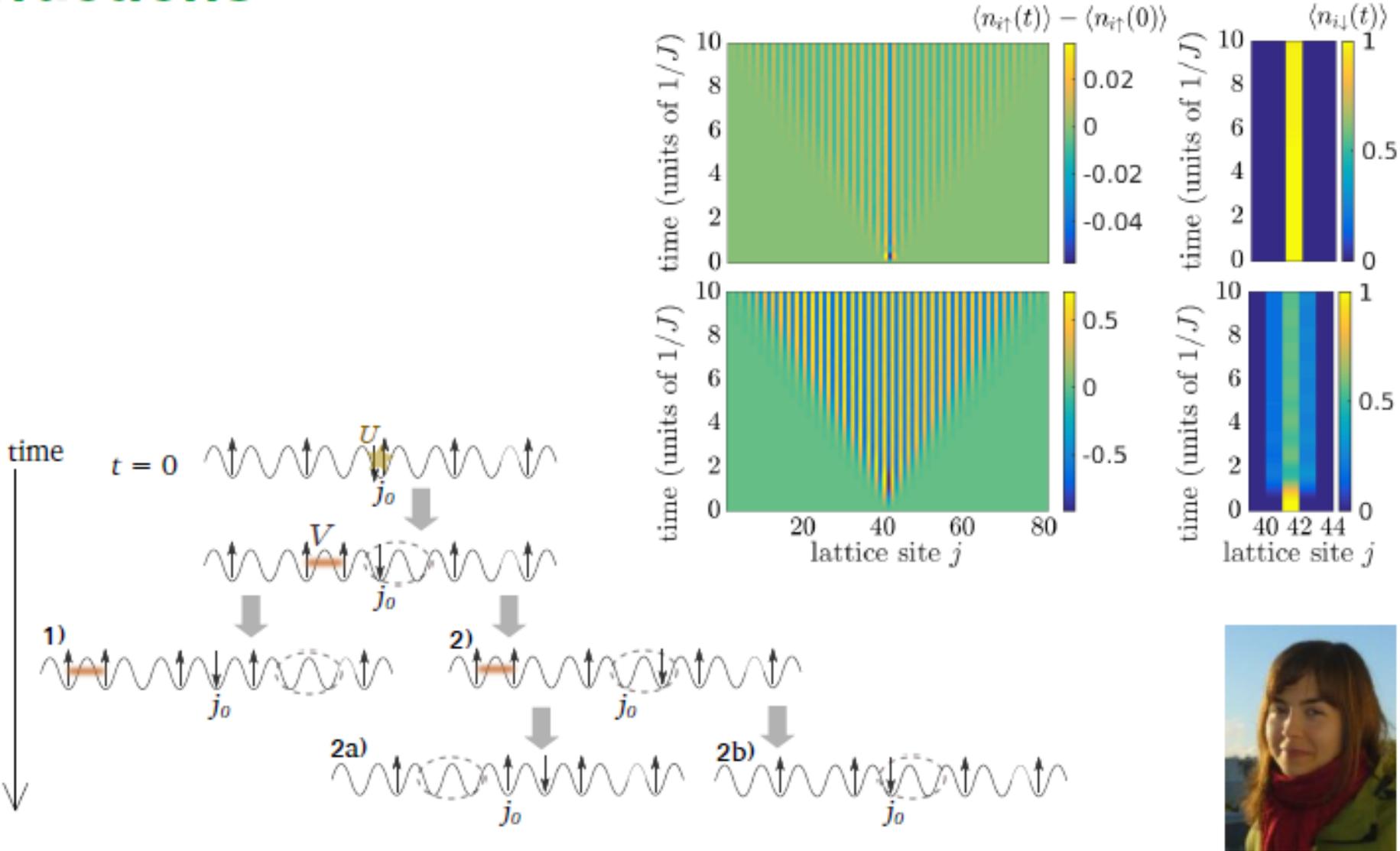


Tuomas Vanhala



Aleksii Julku

# POSTER: Excitations and impurity dynamics in a fermionic Mott insulator with nearest-neighbour interactions



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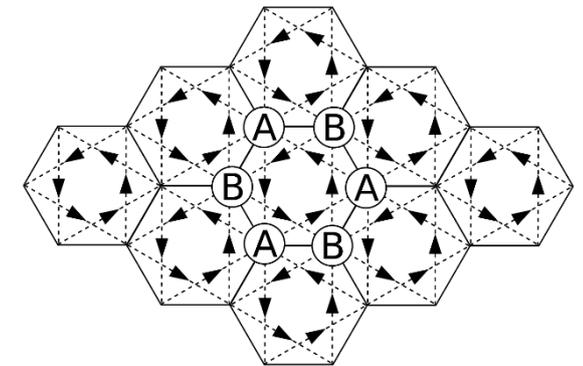
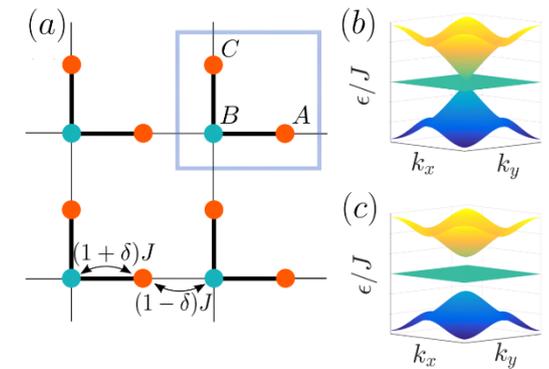
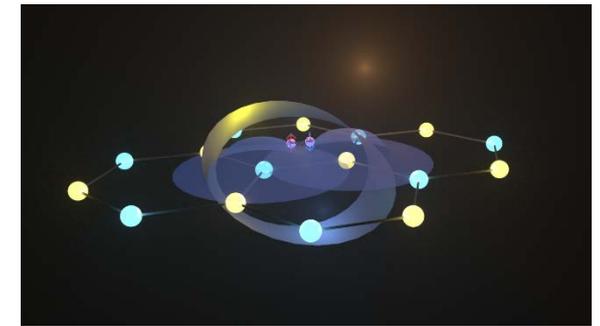
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Sebastiano Peotta



Tuomas Vanhala



Aleksii Julku

# Flat bands: a route to room-temperature superconductivity?

Parabolic band

$$U \ll J \Rightarrow T_c \propto e^{-\frac{1}{U n_0(E_F)}}$$

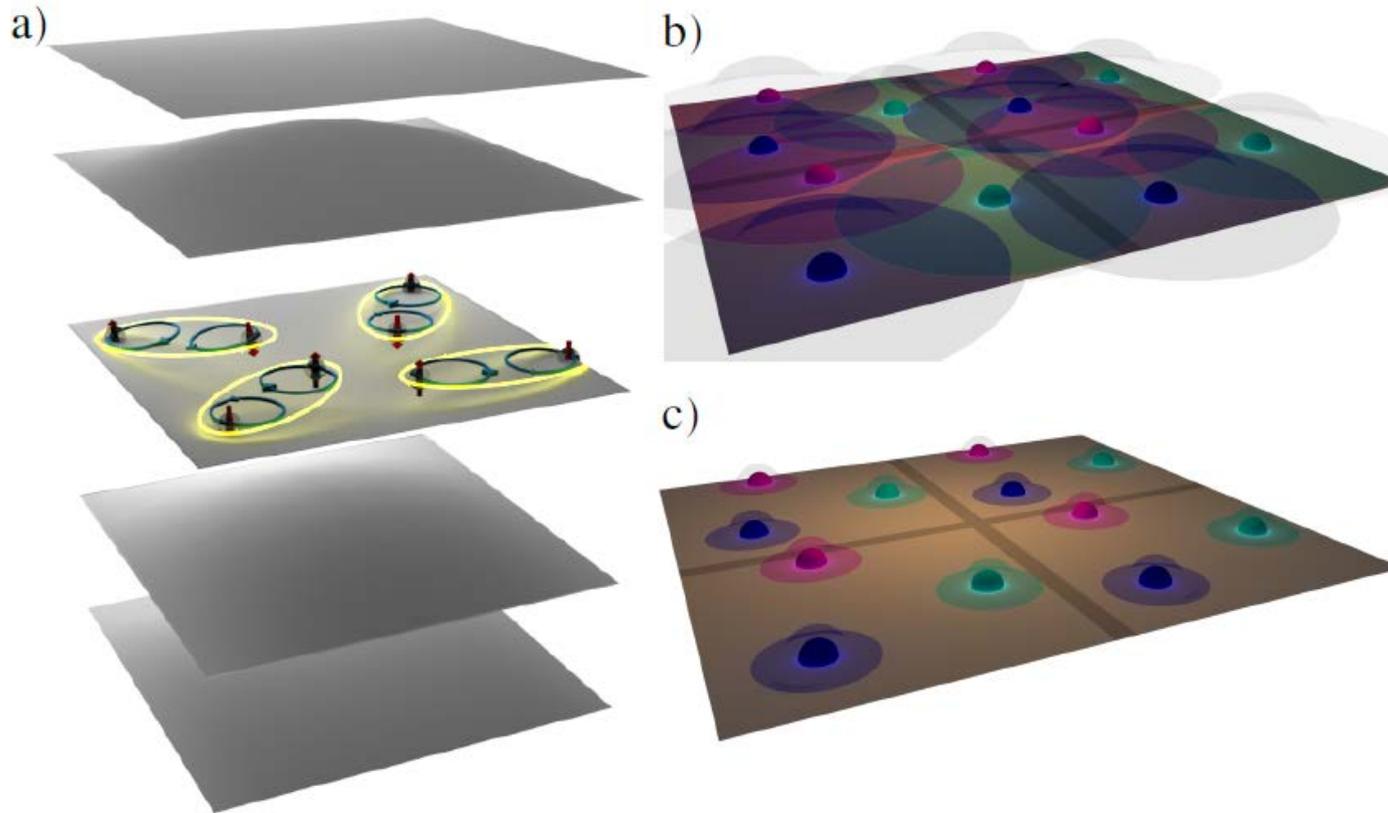
Flat band

$$U \gg J \Rightarrow T_c \propto U n_0(E_F) \propto U/J$$

**Our question:**  
if the band is flat, is there any supercurrent?

**Our answer:**

**yes; superfluid transport is possible in a flat band. It is guaranteed if the band is topologically nontrivial.**



Invariant matrix  $\mathcal{M}_{ij} = \mathcal{M}_{ij}^R + i\epsilon_{ij}C \geq 0$

Real part: superfluid weight

$$D_s$$

Imaginary part: Chern number

$$|C|$$

$$\geq$$

M is Brillouin-zone averaged quantum geometric tensor.

We show that superfluidity and quantum metric are connected!

# Flat bands and room-temperature superconductivity

Parabolic band

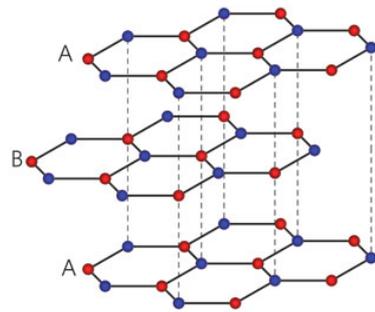
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Flat band

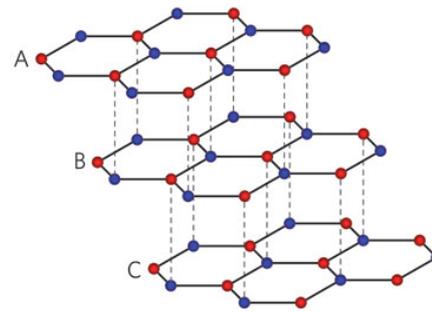
$$U \gg J \Rightarrow T_c \propto U n_0(E_F) \propto U/J$$

a

Trilayer graphene



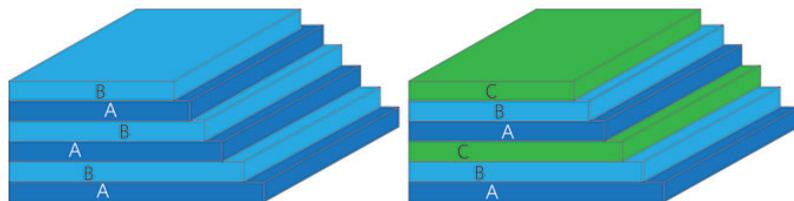
Bernal stacking (ABA)



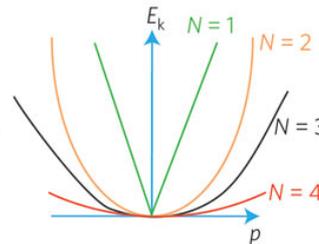
Rhombohedral stacking (ABC)

b

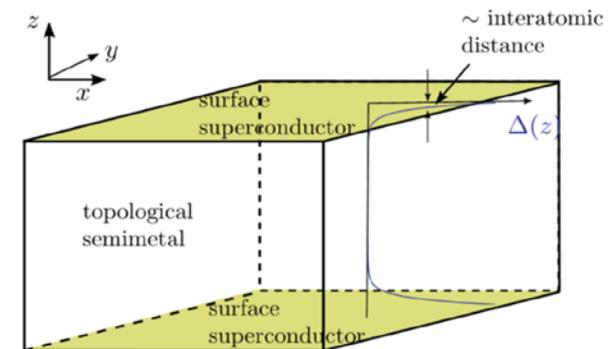
Multilayer graphene



c



Partial flat band of surface states in rhombohedral graphite



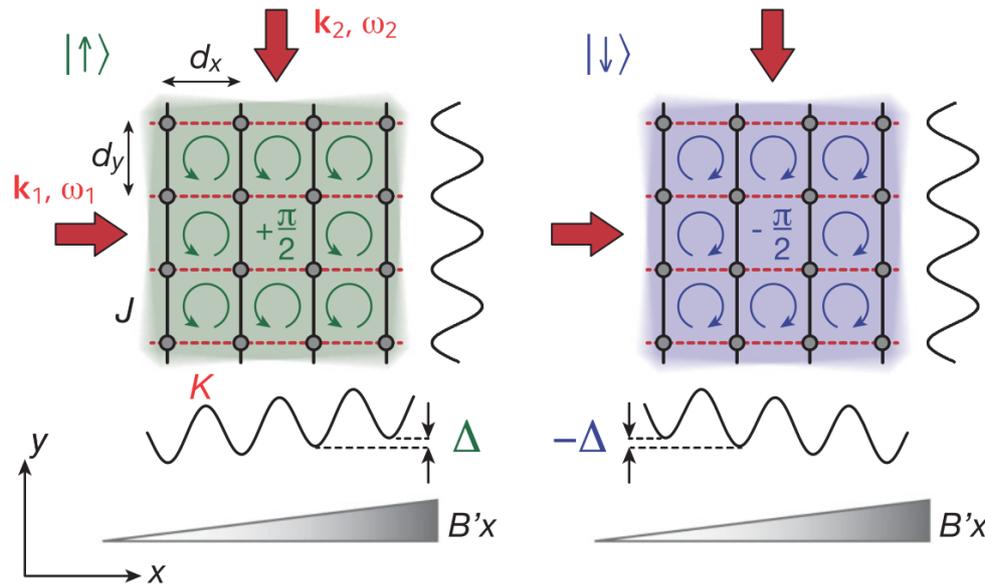
$$T_c \sim g S_{\text{FB}}$$

↑      ↑  
coupling    flat band area

Volovik, J Supercond Nov Magn (2013) 26:2887  
 Kopnin, Heikkilä, Volovik, PRB 83, 220503(R) (2011)  
 Khodel, Shaginyan, JETP Lett. 51, 553 (1990)

# Realization of the Harper Hamiltonian in ultracold gases

$^{87}\text{Rb}$   $|\uparrow\rangle = |F = 1, m_F = -1\rangle$   
 $|\downarrow\rangle = |F = 2, m_F = 1\rangle$



Flux quanta per unit cell  $n_\phi = \frac{1}{7}$

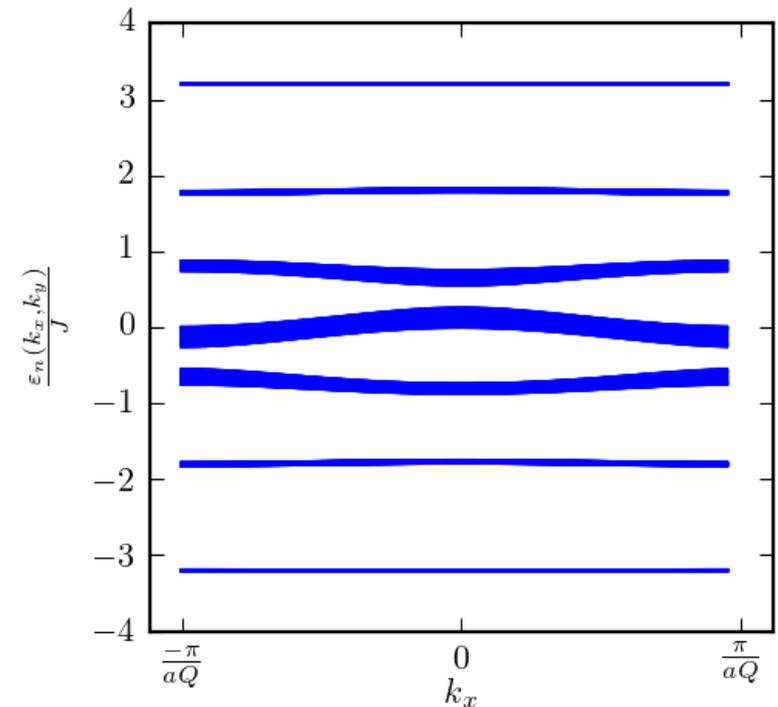


Fig. taken from Ref. 1

- [1] Aidelsburger et al., PRL **111**, 185301 (2013)  
 [2] Miyake et al., PRL **111**, 185302 (2013)

- Time-reversal symmetry is preserved
- Lowest bands are quasi-flat (Landau levels)
- Non-zero Chern number

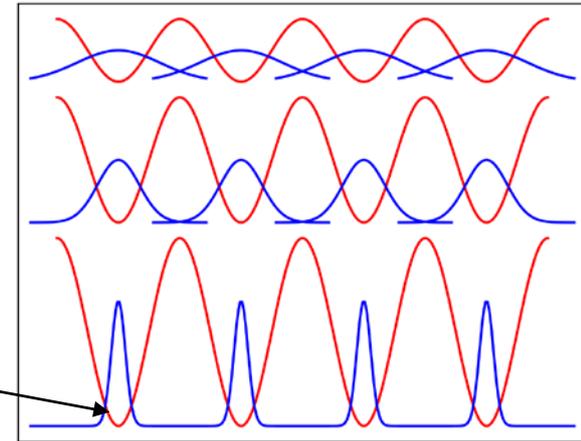
# Superfluid density and superfluid weight

**Nonzero pairing potential** does not guarantee superconductivity

Example of a flat band composed of **localized Wannier functions**

$$\Delta \neq 0$$

$$D_s = 0$$



Definition of superfluid density and superfluid weight

$$\frac{\Delta F}{V} = \frac{1}{2} \rho_s v_s^2 = \frac{1}{2} D_s p_s^2$$

$$v_s = \frac{\hbar \mathbf{q}}{m} \quad \text{Cooper pair velocity}$$

$$2p_s = 2\hbar \mathbf{q} \quad \text{Cooper pair momentum}$$

$$\mathbf{J} = D_s \hbar \mathbf{q} \quad \text{Supercurrent density}$$

$$\left. \begin{array}{l} \Delta \neq 0 \\ D_s \neq 0 \end{array} \right\} \Rightarrow$$



# Superfluid weight from the grand potential

$$[D_s]_{i,j} = \frac{4\pi^2}{Vh^2} \frac{\partial^2 \Omega}{\partial q_i \partial q_j} \Big|_{\mu, \Delta, \mathbf{q}=0}$$

Supercurrent  $\Delta = |\Delta| e^{2iq \cdot r}$

Gauge transformation to make the order parameter real  
and to move  $q$  to the kinetic Hamiltonian (Peierls substitution):

$$K_{i,j} \rightarrow K_{i,j} e^{iq \cdot (r_i - r_j)} \quad K_{i,j} \propto J$$

NOTE: Peierls substitution is justified only if there exist exponentially localized Wannier functions!

# Chern number and Wannier functions

PRL 98, 046402 (2007)

PHYSICAL REVIEW LETTERS

week ending  
26 JANUARY 2007

## Exponential Localization of Wannier Functions in Insulators

Christian Brouder,<sup>1</sup> Gianluca Panati,<sup>2</sup> Matteo Calandra,<sup>1</sup> Christophe Mourougane,<sup>3</sup> and Nicola Marzari<sup>4</sup>

### Theorem:

Exponentially localized Wannier functions can be constructed in 2D or 3D iff the Chern number(s) is zero

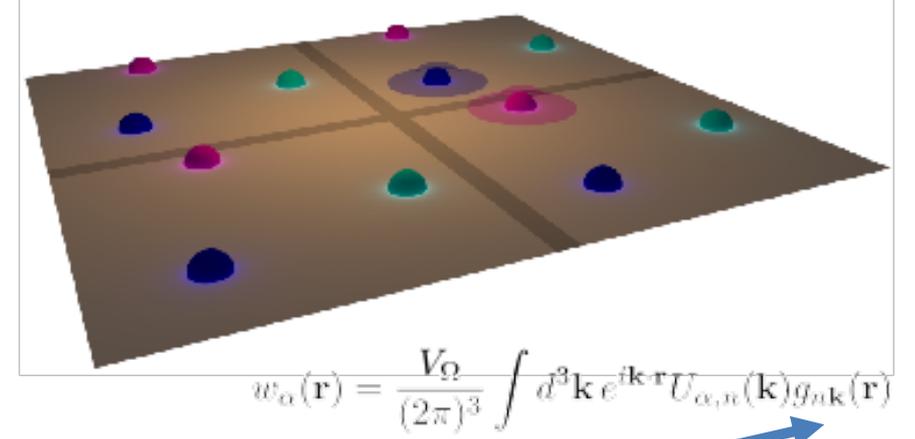
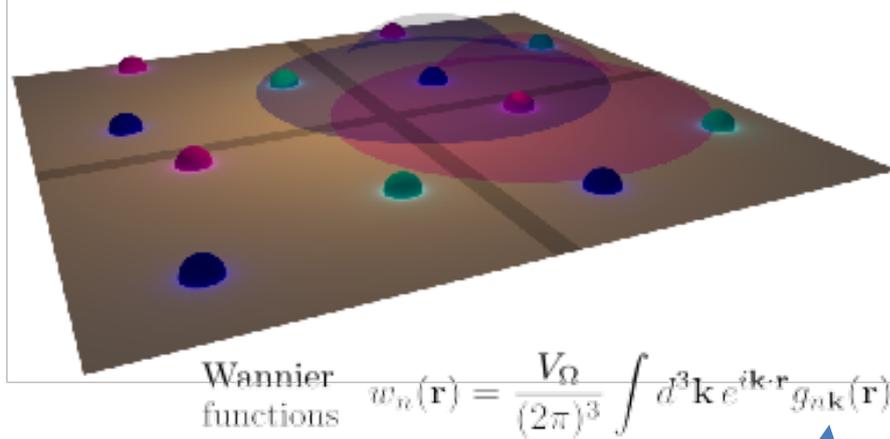
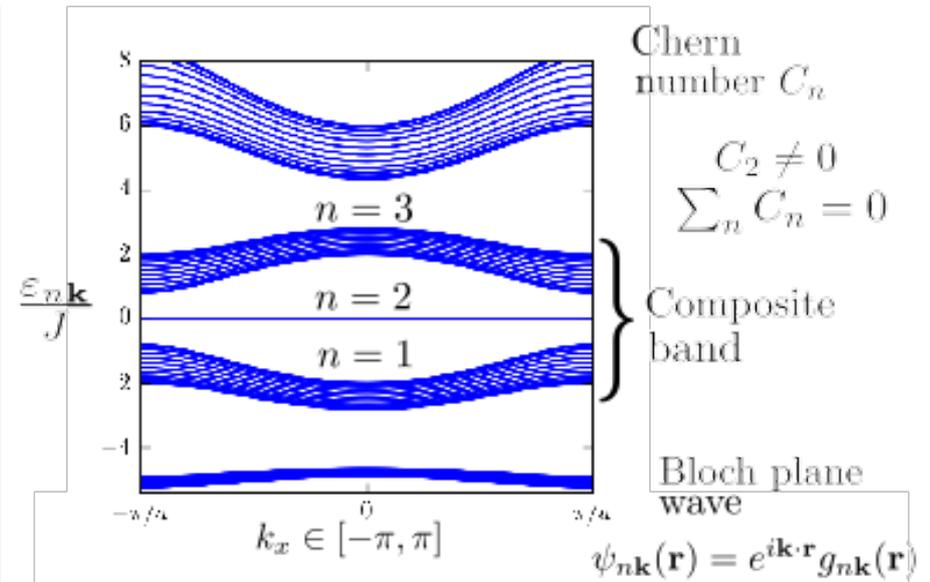
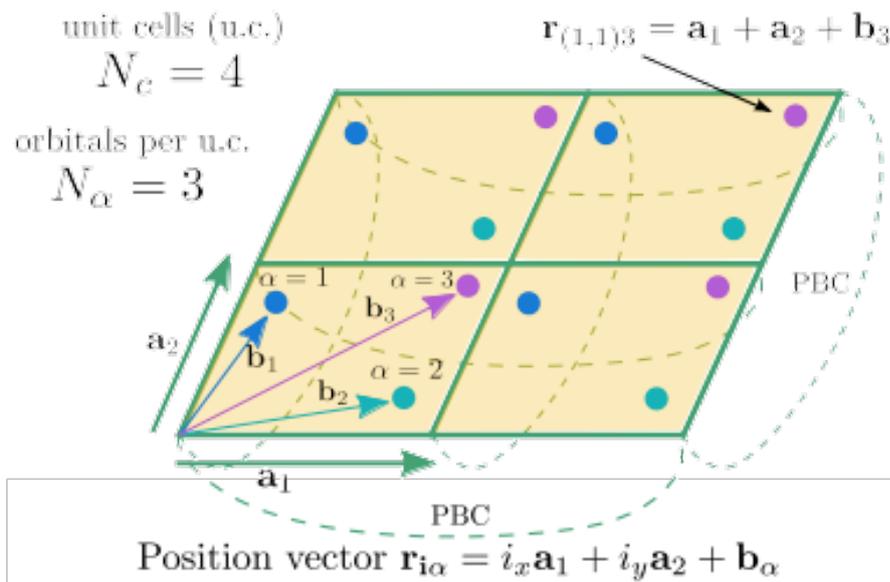
$$\mathbf{A}(\mathbf{k}) = i \langle g_{n\mathbf{k}} | \partial_{\mathbf{k}} g_{n\mathbf{k}} \rangle \quad \text{Berry connection}$$

$$\Omega(\mathbf{k}) = \hat{z} \cdot \nabla \times \mathbf{A}(\mathbf{k}) \quad \text{Berry curvature}$$

$$C = \frac{1}{2\pi} \int_{\text{B.Z.}} d^2\mathbf{k} \Omega(\mathbf{k}) \quad \text{Chern number}$$

Therefore Peierls substitution is not justified for topologically non-trivial (nonzero Chern number) bands.

# The way out: multiband approach



Bloch function for band n

# Superfluid weight in a BCS multiband superconductor

$$\frac{\Delta F}{V} = \frac{1}{2} \rho_s v_s^2 = \frac{1}{2} D_s (\hbar \mathbf{q})^2 \quad [D_s]_{i,j} = \frac{4\pi^2}{V \hbar^2} \frac{\partial^2 \Omega}{\partial q_i \partial q_j} \Big|_{\mu, \Delta, \mathbf{q}=0}$$

$$[\mathcal{G}_{\mathbf{k}}]_{\alpha, n} = g_{n\mathbf{k}\uparrow}(\alpha)$$

Bloch function

$$D_s = D_{s,1} + D_{s,2} + D_{s,3}$$

$$[D_{s,1}]_{i,j} = \frac{2}{V \hbar^2} \sum_{\mathbf{k}} \text{Tr} \left[ \mathcal{V}_{\mathbf{k}} \mathcal{V}_{\mathbf{k}}^\dagger \partial_{k_i} \partial_{k_j} \varepsilon_{\mathbf{k}} \right] \longrightarrow \text{Conventional term present in the single band case}$$

$$\mathcal{D}_{\mathbf{k}}(\mathbf{q}) = -\mathcal{G}_{\mathbf{k}-\mathbf{q}}^\dagger \Delta \mathcal{G}_{\mathbf{k}+\mathbf{q}}$$

$$[D_{s,2}]_{i,j} = \frac{2}{V \hbar^2} \sum_{\mathbf{k}} \text{Tr} \left[ \mathcal{V}_{\mathbf{k}} \mathcal{U}_{\mathbf{k}}^\dagger \partial_{q_i} \partial_{q_j} \mathcal{D}_{\mathbf{k}} \right]$$

$$[D_{s,3}]_{i,j} = \frac{2}{V \hbar^2} \sum_{\mathbf{k}} \sum_{n, n'} \frac{[B_{\mathbf{k},i}]_{n, n'} [B_{\mathbf{k},j}]_{n', n}}{E_{n\mathbf{k}} + E_{n'\mathbf{k}}}$$

$$B_{\mathbf{k},i} = \mathcal{U}_{\mathbf{k}}^\dagger \partial_{q_i} \mathcal{D}_{\mathbf{k}} \mathcal{U}_{\mathbf{k}} + \mathcal{V}_{\mathbf{k}}^\dagger \partial_{q_i} \mathcal{D}_{\mathbf{k}} \mathcal{V}_{\mathbf{k}} + \mathcal{V}_{\mathbf{k}}^\dagger \partial_{k_i} \varepsilon_{\mathbf{k}} \mathcal{U}_{\mathbf{k}} - \mathcal{U}_{\mathbf{k}}^\dagger \partial_{k_i} \varepsilon_{\mathbf{k}} \mathcal{V}_{\mathbf{k}}$$

Geometric term present only in the multiband case

Can be nonzero in a flat band

# Superfluid weight in a flat band

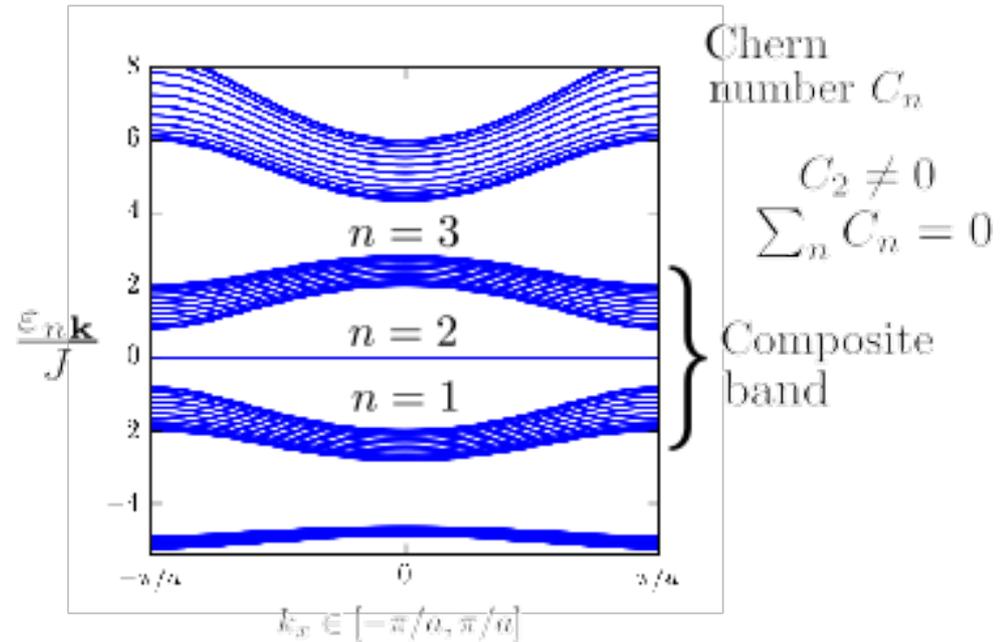
Assumption:  $\Delta_\alpha = \Delta = \text{const.}$

$n_\phi^{-1} = N_\alpha$  Number of orbitals with nonzero pairing order parameter

$\bar{n}$  partially filled flat band

$\nu$  flat band filling

$$\Delta = U n_\phi \sqrt{\nu(1 - \nu)}$$



Isolated flat-band approximation

bandwidth  $J \ll U \ll E_g$  band gap  
 flat band isolated band

### Superfluid weight in a flat band

$$[D_s]_{i,j} = [D_{s,2}]_{i,j} + [D_{s,3}]_{i,j} = \frac{2Un_\phi}{\pi\hbar^2} \nu(1-\nu) \mathcal{M}_{ij}^R$$

Real part of a matrix-valued invariant of the band structure

# QGT

Distance between two nearby quantum states

$$d\ell^2 = g_{ij} ds_i ds_j$$

$$g_{ij} + i\sigma_{ij}$$

Quantum metric

Berry curvature

$$\mathcal{M}_{ij} = \frac{1}{2\pi} \int_{\text{B.Z.}} d^2\mathbf{k} \mathcal{B}_{ij}(\mathbf{k})$$

$$\mathcal{B}_{ij}(\mathbf{k}) = 2\text{Tr}[(\partial_{k_i} \bar{\mathcal{G}}_{\mathbf{k}}^\dagger)(\partial_{k_j} \bar{\mathcal{G}}_{\mathbf{k}})] + 2\text{Tr}[\bar{\mathcal{G}}_{\mathbf{k}}^\dagger(\partial_{k_i} \bar{\mathcal{G}}_{\mathbf{k}})\bar{\mathcal{G}}_{\mathbf{k}}^\dagger(\partial_{k_j} \bar{\mathcal{G}}_{\mathbf{k}})]$$

**We show that the flat band superfluid weight is proportional to the Brillouin-zone averaged quantum metric, and derive a lower bound to it**

$$\mathcal{M}_{ij} = \mathcal{M}_{ij}^R + i\epsilon_{ij} C \geq 0 \Rightarrow \det(\mathcal{M}^R) \geq |C|^2$$

Chern number

$$D_s \geq |C|$$

# Parabolic band vs. flat band

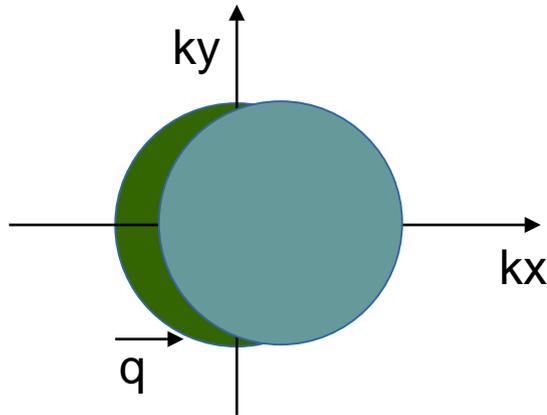
## Parabolic band

$$D_s = \frac{n_p}{m_{\text{eff}}} \left( 1 - \left( \frac{2\pi\Delta}{k_B T} \right)^{1/2} e^{-\Delta/(k_B T)} \right)$$

$$\frac{1}{m_{\text{eff}}} \propto J$$

Particle density  $n_p$   
Bandwidth

Physical picture: global shift of the Fermi surface



## Flat band

$$[D_s]_{i,j} = \frac{2U n_\phi}{\pi \hbar^2} \nu (1 - \nu) \mathcal{M}_{ij}^R$$

Linearly proportional to the coupling constant  $U$ !

Physical picture:

Delocalization of Wannier functions

Overlapping Cooper pairs: pairing fluctuations support transport if pairs can be created and destroyed at distinct locations

## Riemannian Structure on Manifolds of Quantum States

J. P. Provost and G. Vallee

Physique Theorique, Universite de Nice\*. \*\*

$$\langle \quad | \quad \rangle$$
$$\|\psi(s + ds) - \psi(s)\|^2 = (\partial_i \psi, \partial_j \psi) ds_i ds_j \left( \partial_i = \frac{\partial}{\partial s_i} \right)$$

$$(\partial_i \psi, \partial_j \psi) = \gamma_{ij} + i\sigma_{ij}$$

Gauge invariant version:

$$g_{ij}(s) = \gamma_{ij}(s) - \beta_i(s) \beta_j(s) \quad \beta_j(s) = -i(\psi(s), \partial_j \psi(s))$$

Distance between two nearby quantum states

$$d\ell^2 = g_{ij} ds_i ds_j$$

### QGT

$$g_{ij} + i\sigma_{ij}$$

Quantum metric

Berry curvature

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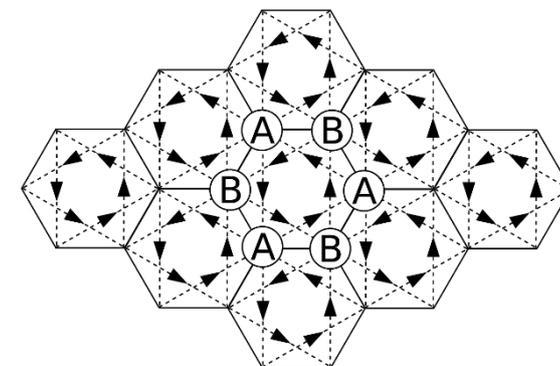
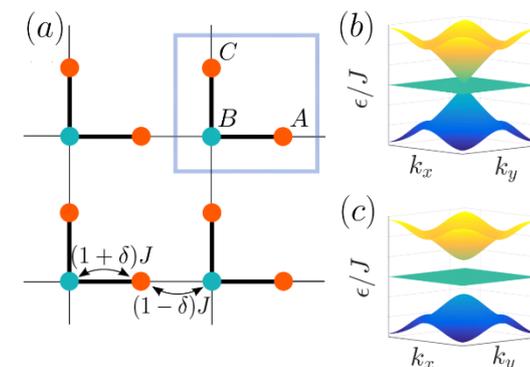
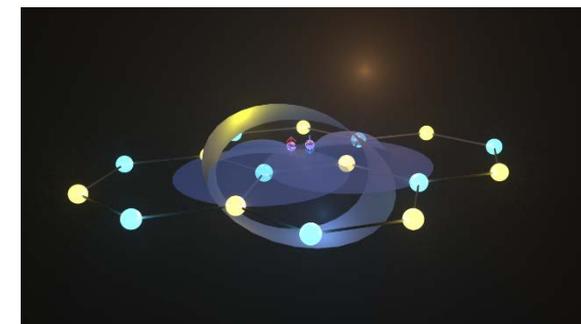
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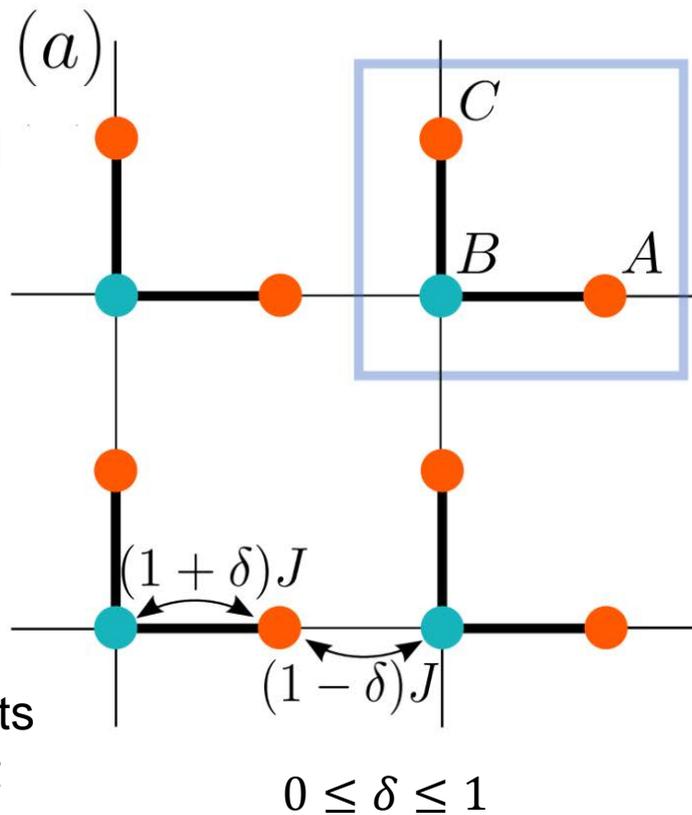


Aleksii Julku

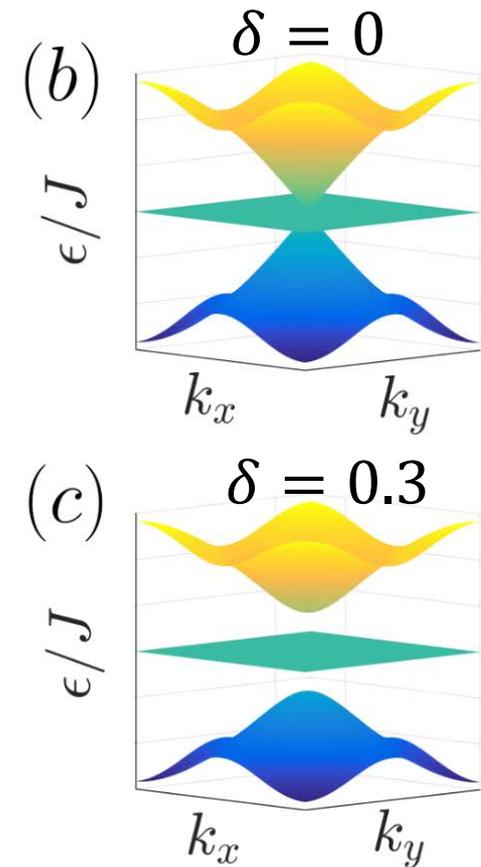
# Lieb lattice

What about superfluidity in topologically trivial flat bands?

Three bands: two dispersive and one strictly flat band with  $C = 0$



Staggered hopping coefficients enable the isolation of the flat band



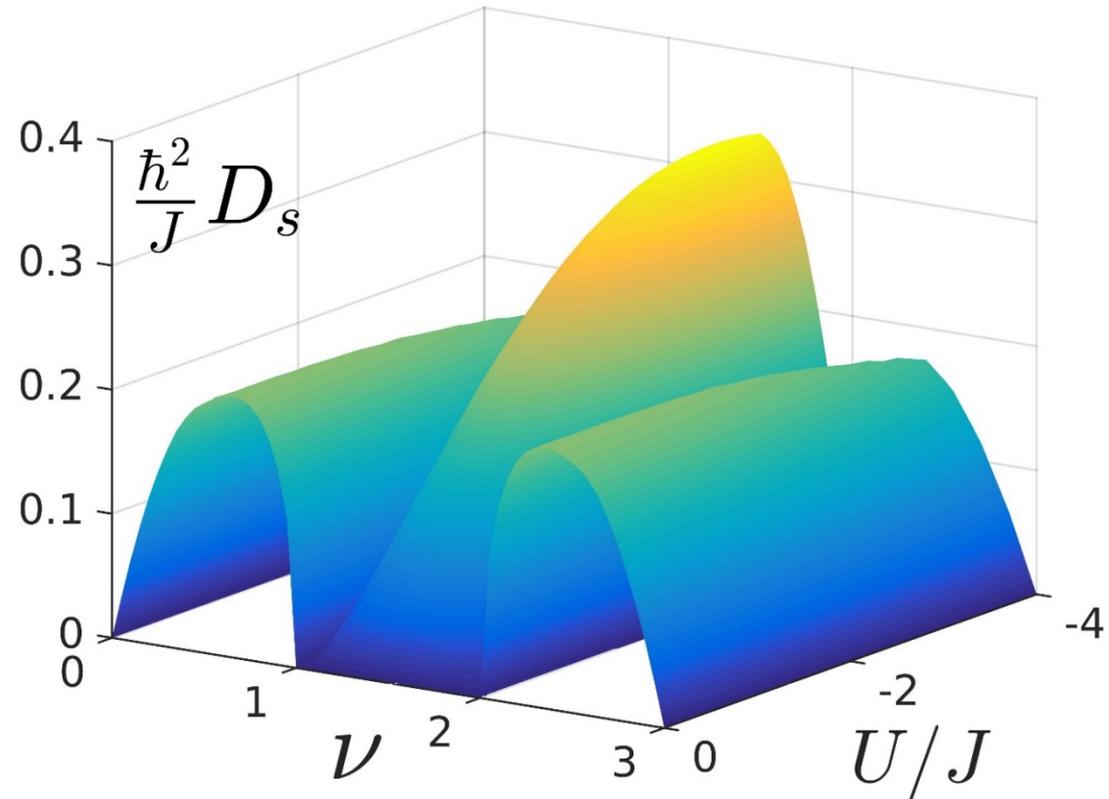
# Lieb lattice: superfluid weight

$\nu$  Total filling ( $1 < \nu < 2$  for the flat band)

$D_s$  on the flat band depends strongly on  $U$

$D_s$  on dispersive bands roughly constant

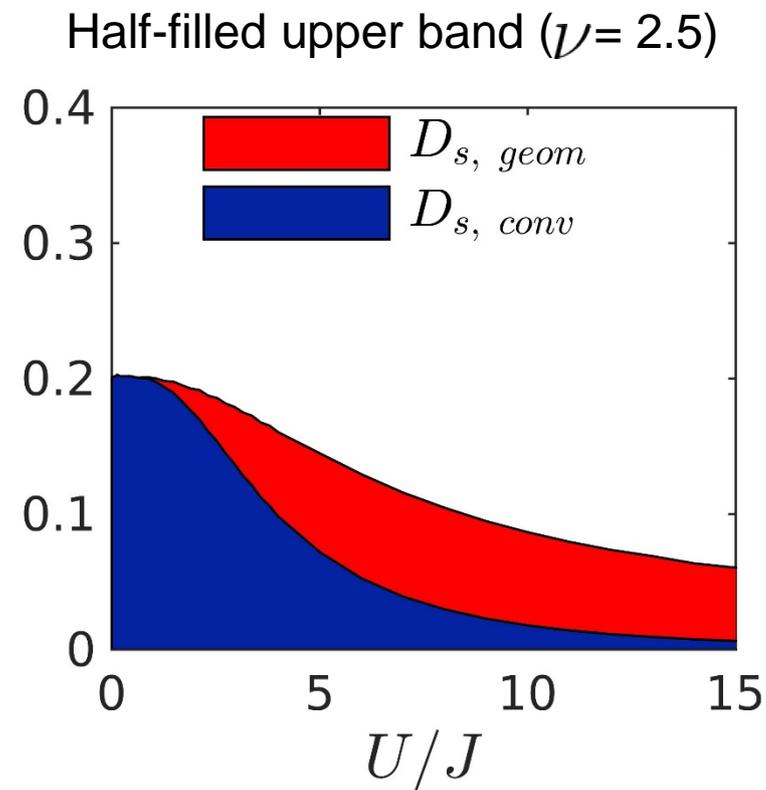
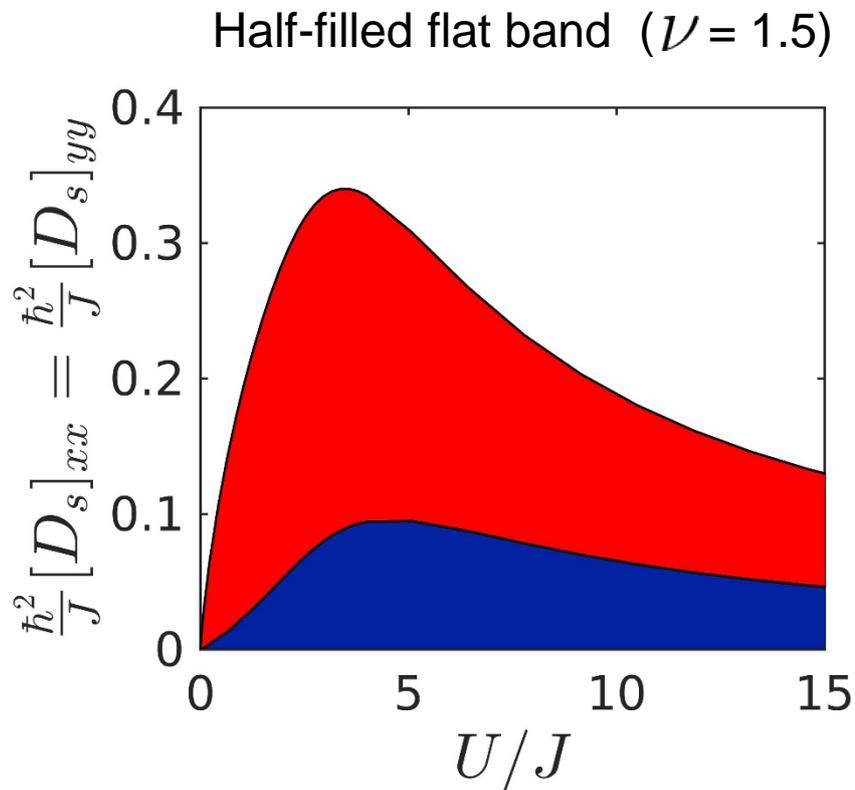
$D_s$  for the trivial flat bands is non-zero and large!



# Lieb lattice: geometric contribution

Large  $D_s$  and its strong dependence on  $U$  within the flat band is explained by the geometric superfluid weight contribution

$$D_{s,geom} = D_{s,2} + D_{s,3}$$



# For isolated flat band, the BCS wavefunction is exact!

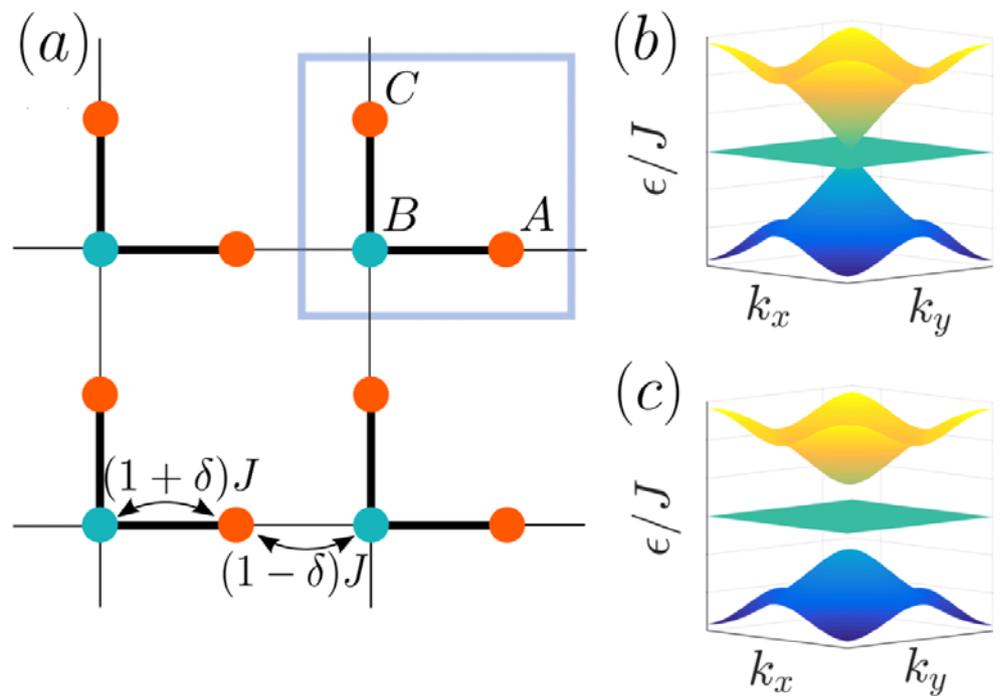
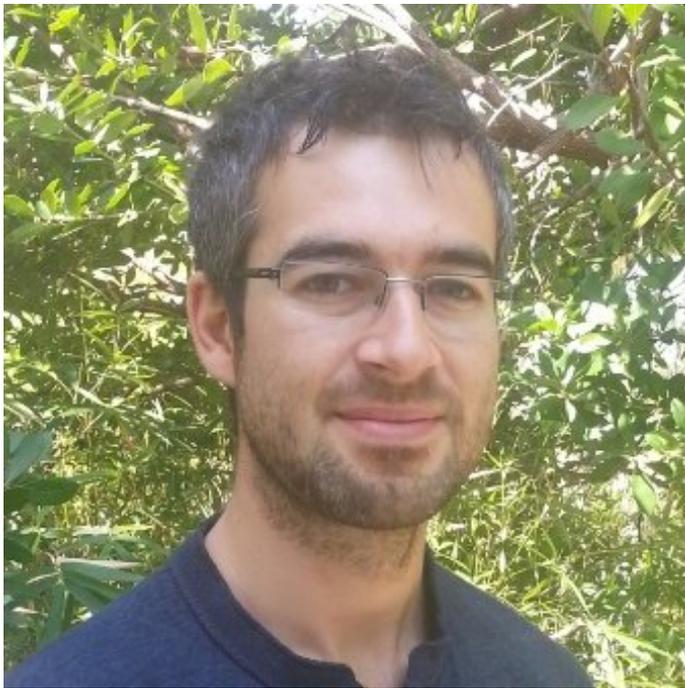
(for bipartite lattices)

The mean-field prediction of finite flat band superfluidity is exact for bipartite lattices and isolated flat bands.

For partially flat bands we have confirmed the results by DMFT and ED.

# See POSTER 30 on the Lieb lattice superfluidity

Sebastiano Peotta



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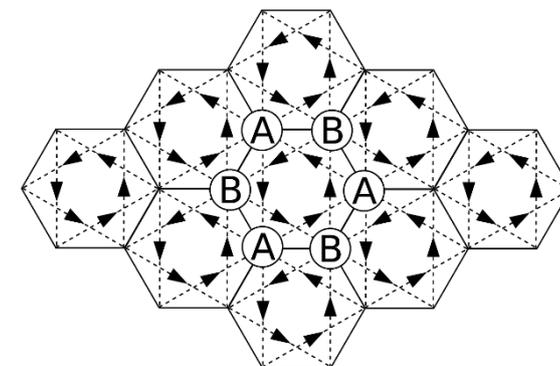
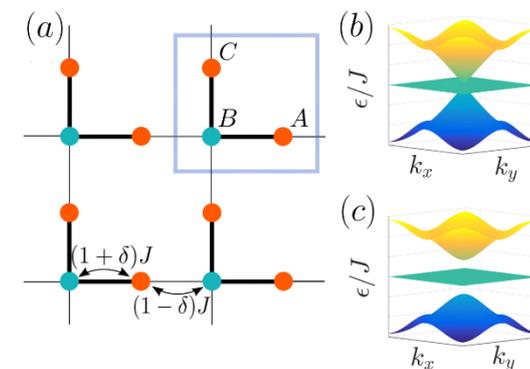
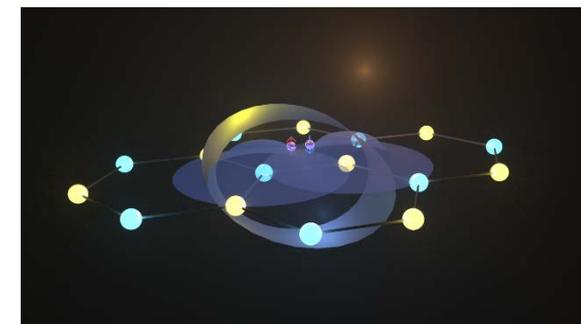
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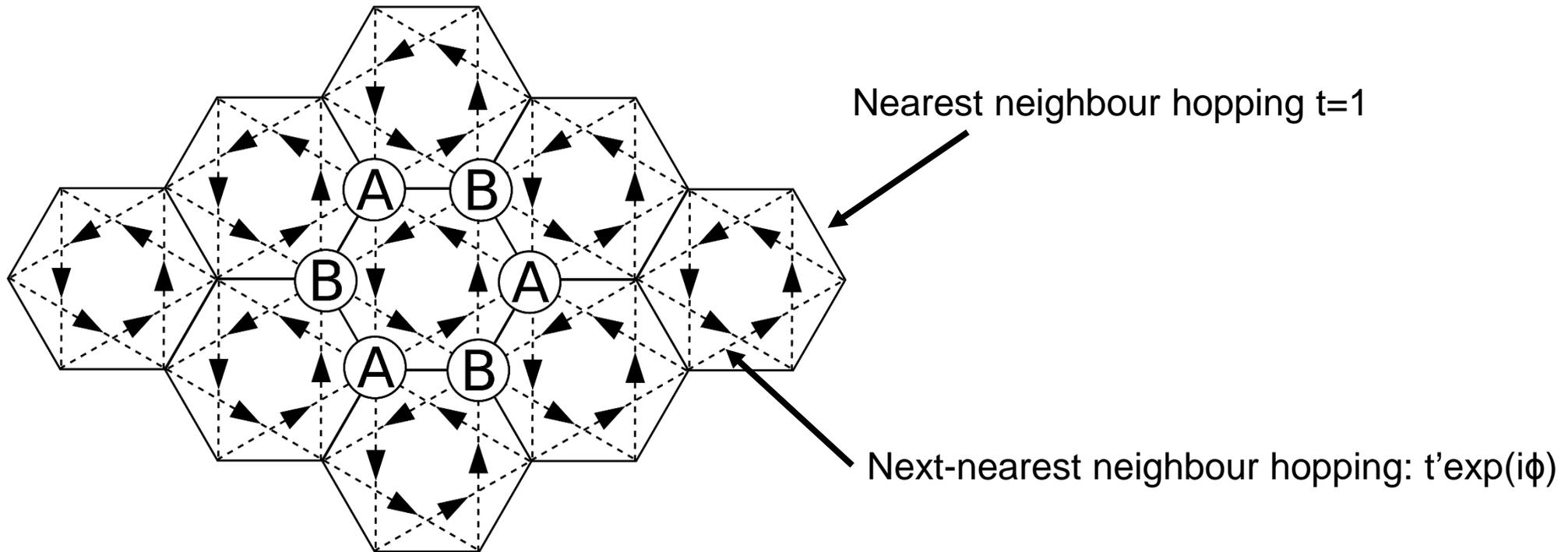
Tuomas Vanhala



Aleksii Julku

# Haldane-Hubbard model

Potential difference  $\Delta_{AB}$  between the sublattices



Noninteracting model a well known model of a **topological insulator**

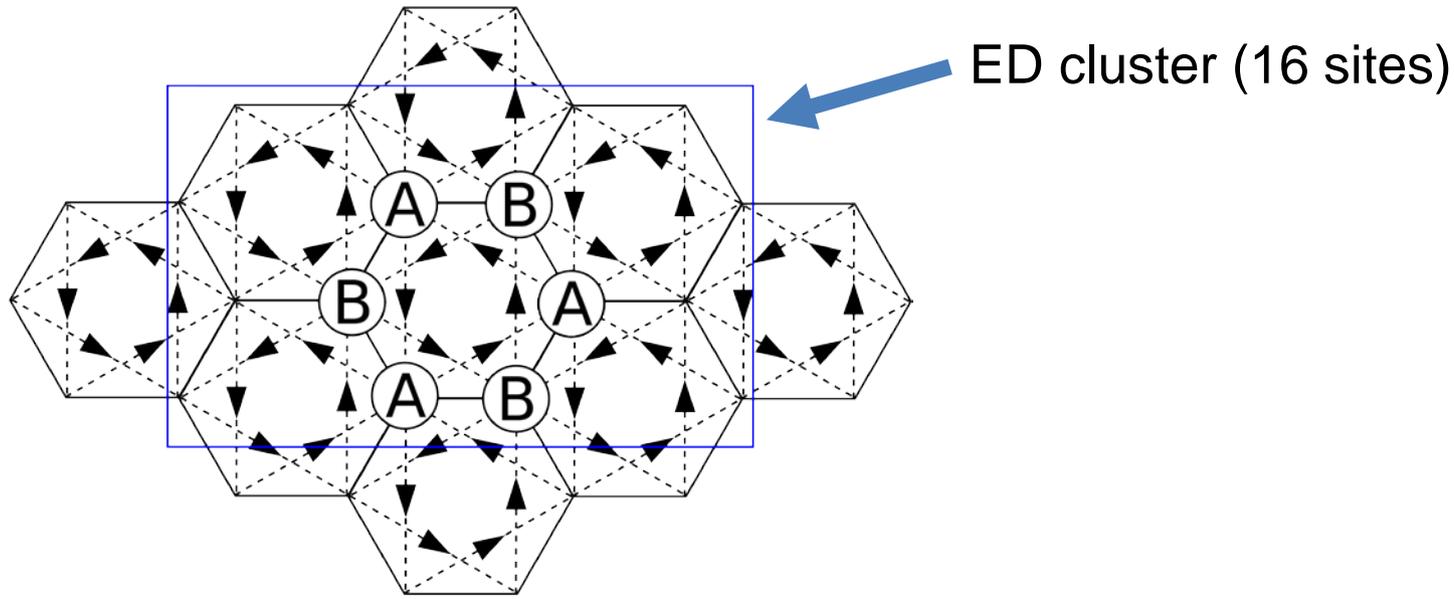
Gotzke et al., Nature **515**, 237 (2014)

Take a two-component version:

**What are the effects of an on-site Hubbard repulsion?**

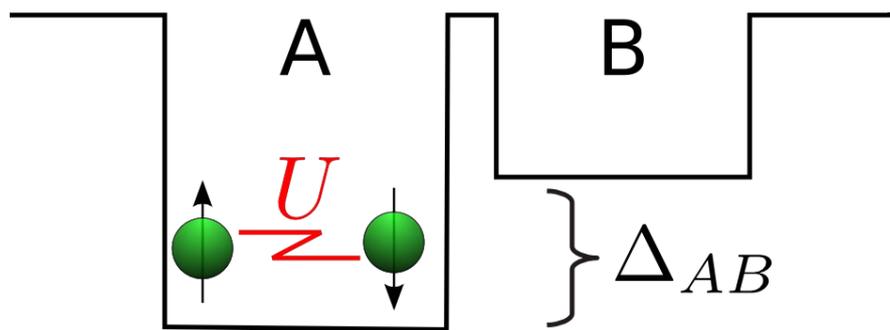
Mean field: Physica B 481, 53-58; PRB 84, 035127; PRB 85, 205107; J. Phys B. 26, 175601  
Feng, Kou, Huber groups

# Exact diagonalization and DMFT: two complementary methods

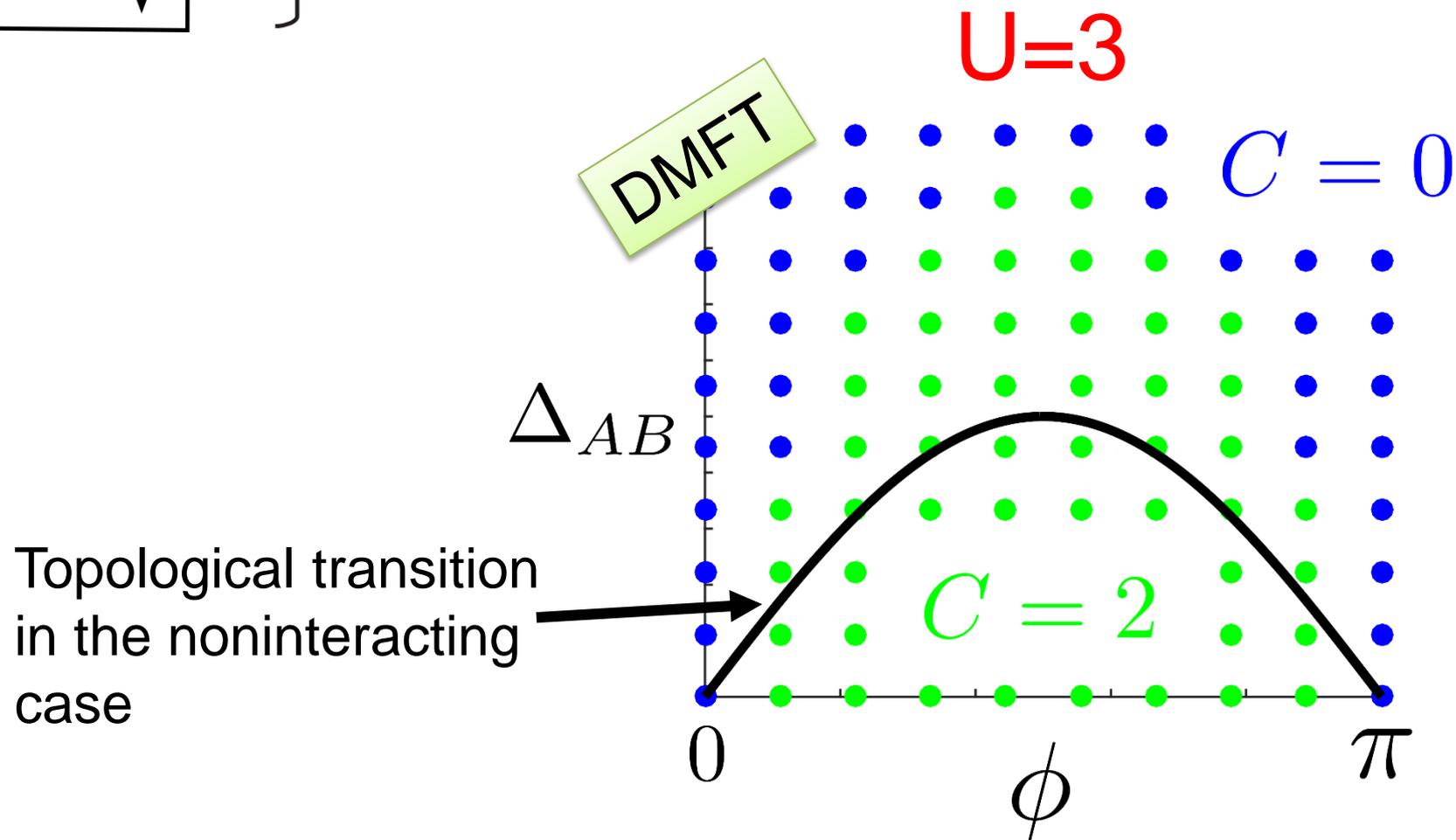


- ED: Finite system, but correlations treated exactly
  - Can map out topological phase boundaries using twisted boundary conditions
- DMFT: Thermodynamic limit, but only local quantum correlations treated exactly
  - Chern numbers using the "topological Hamiltonian" (Z. Wang and S.-C. Zhang, Phys. Rev. X 2, 031008, 2012)

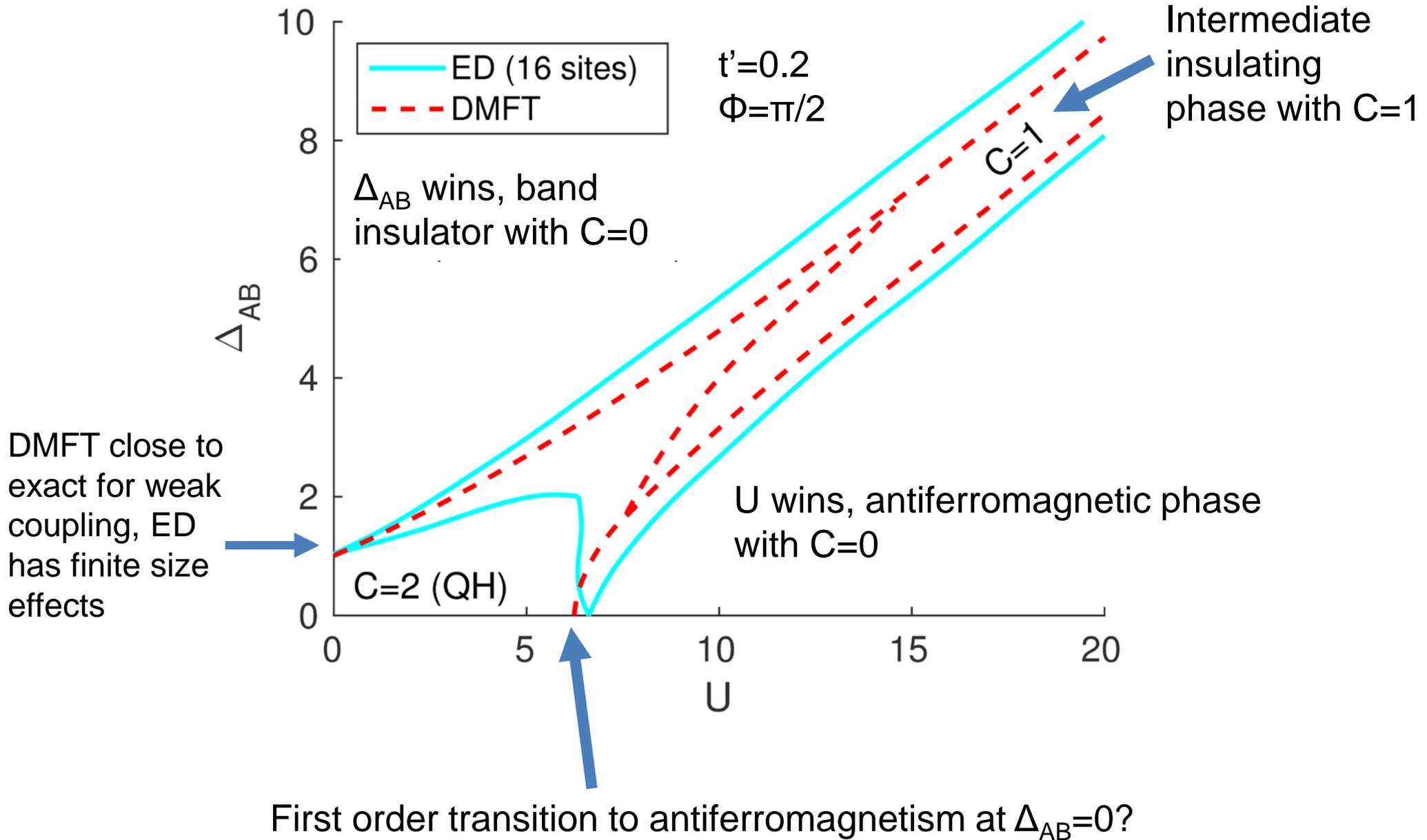
# Interactions oppose the effect of the sublattice potential difference



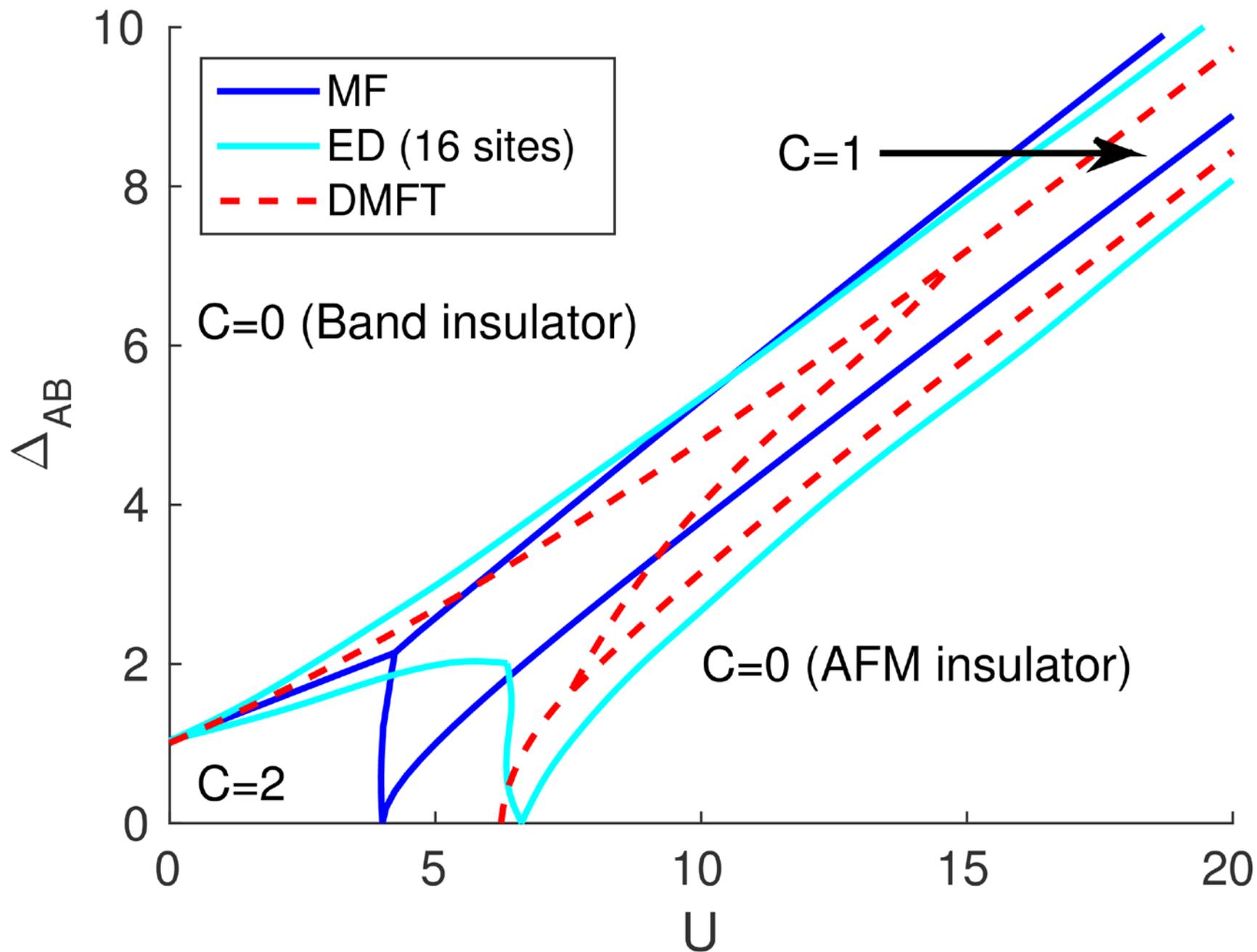
Weak interactions: Enlarged topological phase



# Strong interactions: $U$ drives antiferromagnetism, $\Delta_{AB}$ density wave



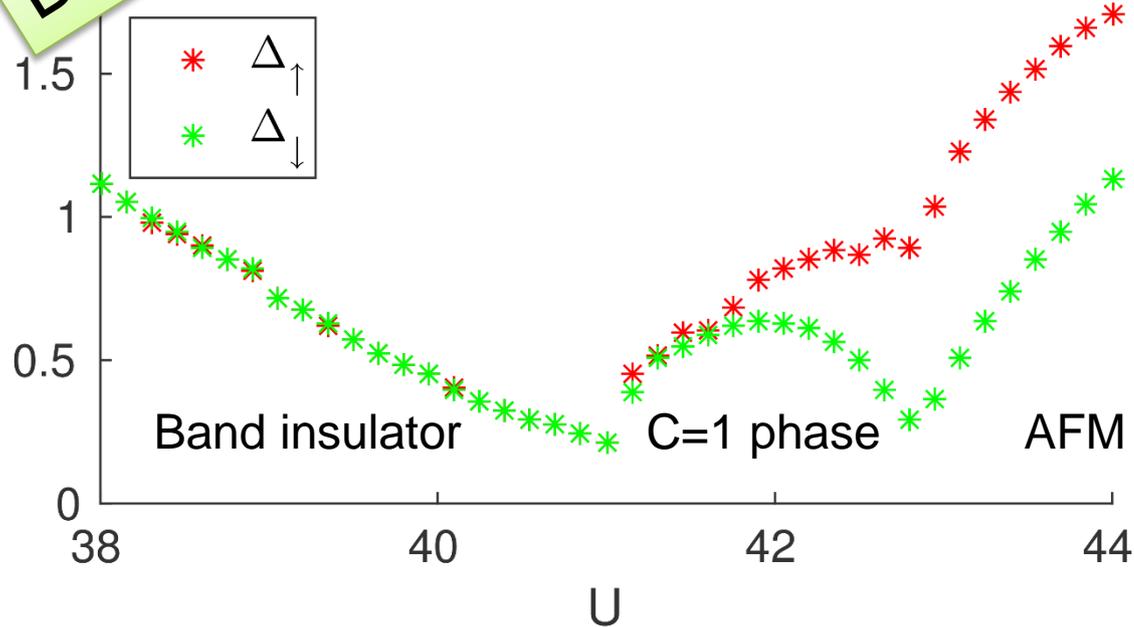
## Comparison with pure mean field



# Intermediate insulating phase with $C=1$

DMFT

Single particle gaps at  $\Delta_{AB} = 20$



One spin component in the quantum Hall phase, the other one in the band insulating (density wave) phase.

arXiv:1512.08804

Geometry and topology make superfluidity possible even in flat bands

Chern number  $C=1$  phase in the Haldane-Hubbard model

## Summary

