Aalto University
School of Science

Quantum geometry effects on superconductivity, Bose-Einstein condensation, and light-matter interactions in flat bands

Päivi Törmä

Aalto University

IBS Conference on Flatbands: symmetries, disorder, interactions and thermalization, South Korea (on-line)

17.8.2021

PREIN

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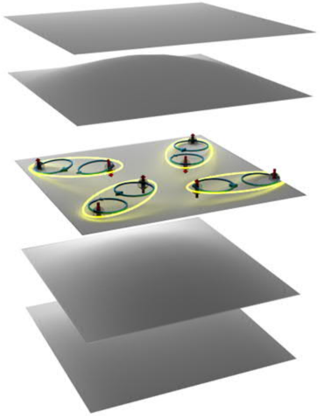
<u>Quantum geometry and superconductivity</u>

- **Can we reach room temperature superconductivity?**
- **What does quantum geometry have to do with this?**

<u>Quantum geometry and BEC</u>

<u>Quantum geometry and light-matter interactions</u>



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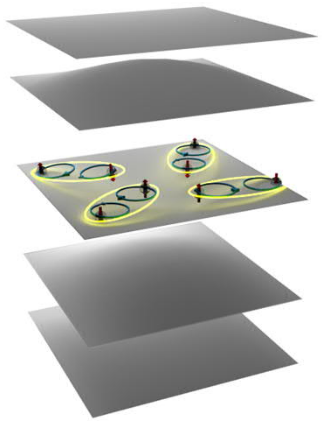
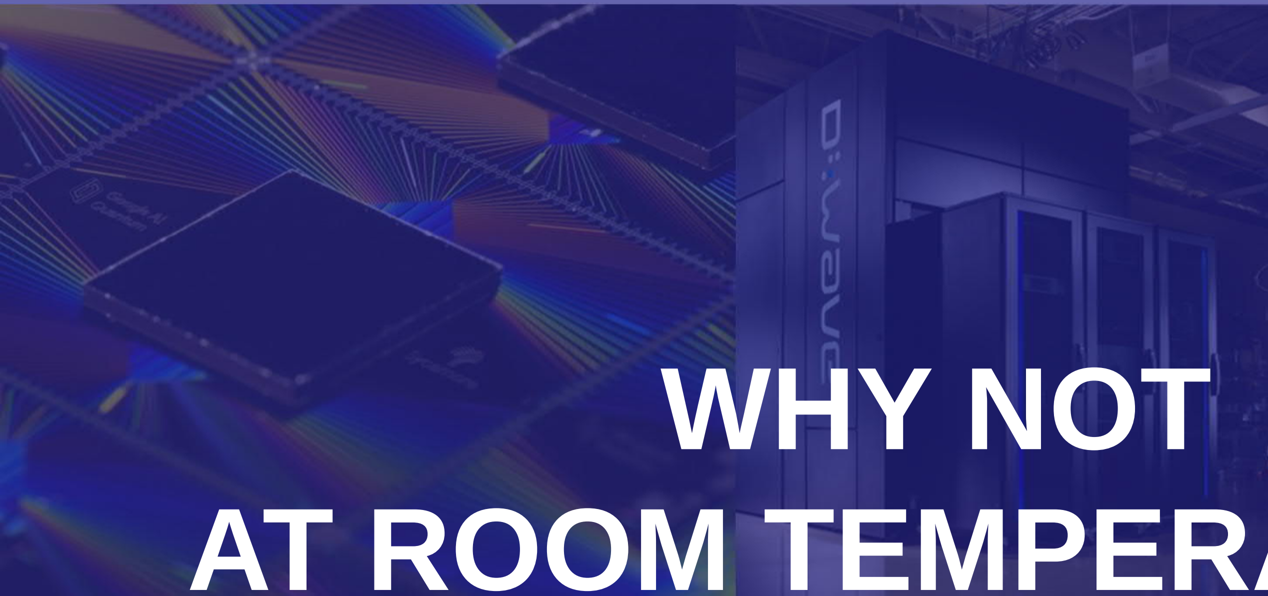
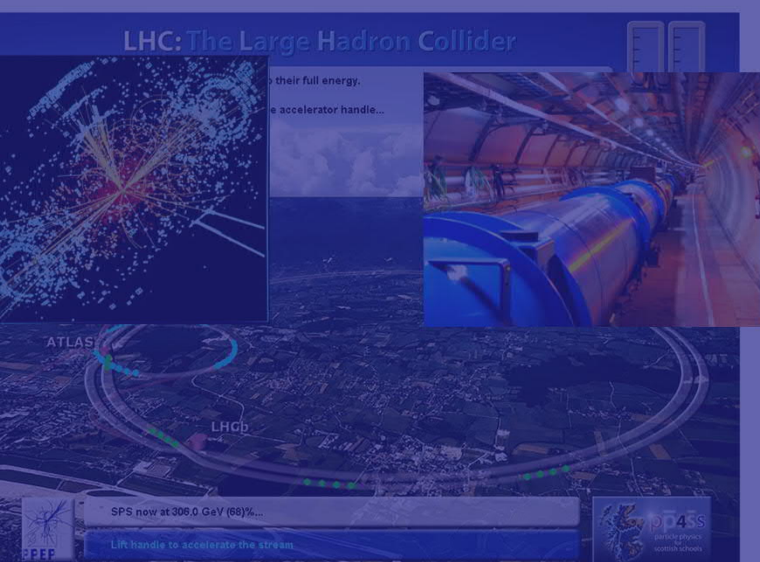


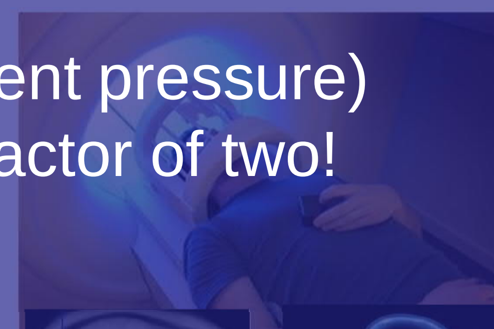
SUPERCONDUCTIVITY



WHY NOT
AT ROOM TEMPERATURE?



Highest T_c (ambient pressure)
~150 K – just a factor of two!



Superconductivity: BEC of Cooper pairs

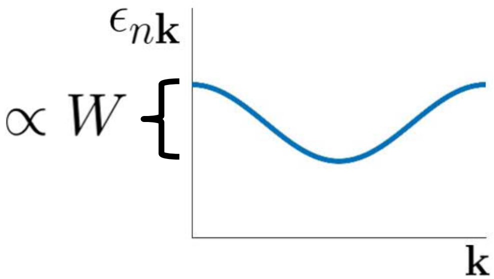
Weak interaction U
Large kinetic energy (Fermi level)
Low critical temperature

$$T_c \propto e^{-1/(U n_0(E_f))}$$

Remove the kinetic energy to maximize the effect of interactions!

Flat bands: interactions dominate

Dispersive band U<<W:



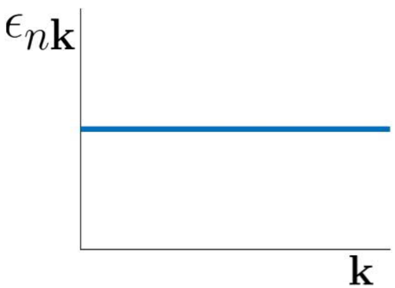
$$\psi_n(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$

(periodic part of) the Bloch function

T_c for Cooper pairing

$$T_c \propto e^{-1/(U n_0(E_f))}$$

Flat band U>>W:



$\epsilon_{n\mathbf{k}} =$ constant

Group velocity: $\frac{\partial \epsilon_{n\mathbf{k}}}{\partial k} = 0$

No interactions: insulator at any filling

$$T_c \propto U V_{\text{flat band}}$$

High T_c for pairing
(Khodel, Shaginyan, Volovik, Kopnin, Heikkilä)

But is supercurrent stable at a flat band?

Supercurrent density: given by superfluid weight and Cooper pair momentum

$$\mathbf{J} = \frac{1}{4} D_s \hbar \mathbf{q}$$

Conventional BCS: $D_s = \frac{n_{\mathrm{p}}}{m_{\mathrm{eff}}} \left(1 - \left(\frac{2\pi\Delta}{k_{\mathrm{B}}T} \right)^{1/2} e^{-\Delta/(k_{\mathrm{B}}T)} \right)$

Zero at a flat band!!!

n_{p} Particle density

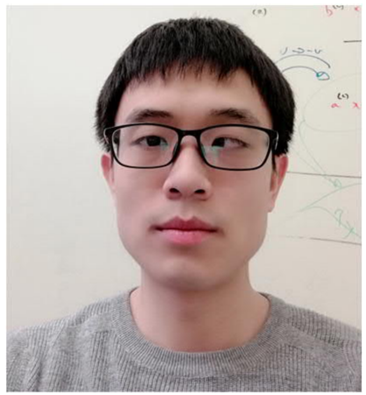
$$\frac{1}{m_{\mathrm{eff}}} \propto J \propto \partial_{k_i} \partial_{k_j} \epsilon_{\mathbf{k}}$$

Bandwidth

$i, j = x, y, z$

Superfluidity and quantum geometry

Sebastiano Peotta



Long Liang

Sebastian
Huber

Murad
Tovmasyan

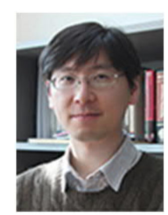
Aleksi
Julku

Tuomas
Vanhala

Peotta, PT, Nat Comm 2015
Julku, Peotta, Vanhala, Kim, PT, PRL 2016
Tovmasyan, Peotta, PT, Huber, PRB 2016
Liang, Vanhala, Peotta, Siro, Harju, PT, PRB 2017
Liang, Peotta, Harju, PT, PRB 2017
Tovmasyan, Peotta, Liang, PT, Huber, PRB 2018
PT, Liang, Peotta, PRB(R) 2018

Ari Harju

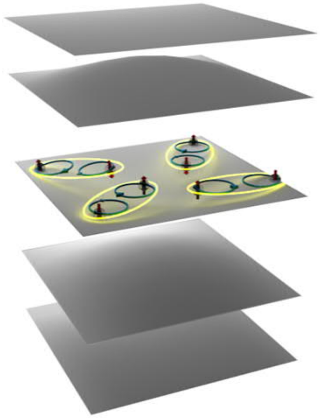
Topi Siro



Dong-Hee Kim

Our multiband approach

MULTIBAND BCS MEAN-FIELD THEORY
multiband two-component attractive
Fermi-Hubbard model –U < 0



$$H = -\sum_{ij\alpha\beta\sigma} t^{\sigma}_{i\alpha j\beta} c^{\dagger}_{i\alpha\sigma} c_{j\beta\sigma} - U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} - \mu \sum_{i\alpha\sigma} n_{i\alpha\sigma}$$

Introduce a modulation of the order parameter phase to generate supercurrent

$$\Delta(\mathbf{r}) \to \Delta(\mathbf{r}) e^{2i\mathbf{q}\cdot\mathbf{r}}$$

$2\mathbf{q}$: Cooper pair momentum

$$[D_s]_{ij} \propto \left. \frac{\partial^2 \Omega}{\partial q_i \partial q_j} \right|_{\mathbf{q}=0}$$

$$i, j = x, y, z$$

$$\mathbf{j}(\mathbf{q}, \omega) = K(\mathbf{q}, \omega) \mathbf{A}(\mathbf{q}, \omega)$$

$$D_s = \lim_{\mathbf{q}\to 0} K(\mathbf{q}, \omega = 0)$$

Superfluid weight in a multiband system

$$D_s = D_{s,\mathrm{conventional}} + D_{s,\mathrm{geometric}}$$

$$i, j = x, y, z$$

$$\propto \partial_{k_i} \partial_{k_j} \epsilon_{\mathbf{k}}$$

Can be nonzero also in a flat band
Present only in a multiband case
Proportional to the quantum metric

$$[D_{s,\mathrm{geometric}}]_{ij} \propto U g_{ij}$$

Quantum geometric tensor

Metric for the distance between quantum states

$$d\ell^2 = ||u(\mathbf{k}+d\mathbf{k}) - u(\mathbf{k})||^2 = \langle u(\mathbf{k}+d\mathbf{k}) - u(\mathbf{k})|u(\mathbf{k}+d\mathbf{k}) - u(\mathbf{k})\rangle$$

$$\approx \sum_{i,j} \underbrace{\langle \partial_{k_i} u | \partial_{k_j} u\rangle}_{} dk_i dk_j$$

Introduce gauge invariant version $\left(u(\mathbf{k}) \leftrightarrow u(\mathbf{k})e^{i\phi(\mathbf{k})}\right)$

Quantum geometric tensor

$$\mathcal{B}_{ij}(\mathbf{k}) = 2\langle \partial_{k_i} u|(1 - |u\rangle\langle u|)|\partial_{k_j} u\rangle$$

$$\mathrm{Re}\,\mathcal{B}_{ij} = g_{ij}$$ quantum metric $d\ell^2 = \sum_{ij} g_{ij} dk_i dk_j$

$$\mathrm{Im}\,\mathcal{B}_{ij} = [\mathbf{\Omega}_{\mathrm{Berry}}]_{ij}$$ Berry curvature

Provost, Vallee, Comm. Math. Phys. **76**, 289 (1980)

Quantum metric is the same as Fubini-Study metric,
and related to Fisher information

Lower bound for flat band superfluidity

The quantum geometric tensor $\mathcal{B}_{ij}$
is complex positive semidefinite

$$\Rightarrow \boxed{D_s \geqslant \int_{B.Z.} d^d\mathbf{k} |\mathbf{\Omega}_{\mathrm{Berry}}(\mathbf{k})| \geqslant C}$$

Berry curvature: $\Omega(\mathbf{k}) = i\hat{z} \cdot \nabla \times \langle u_{n\mathbf{k}} | \partial_{\mathbf{k}} u_{n\mathbf{k}} \rangle$

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

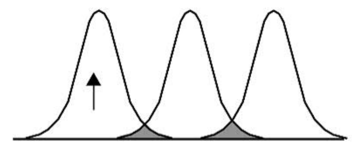
Mean-field results confirmed by:
exact diagonalization, DMFT, DMRG, perturbation theory

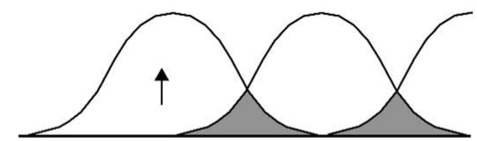
Why can there be transport in a flat band?

Overlap of the Wannier functions
Multiband processes

Single flat band

Multiband system with a flat band

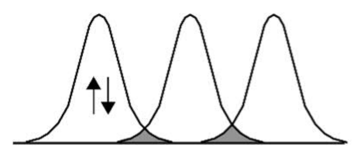


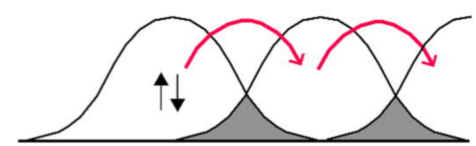


transport ~0

transport ~0 due to geometry or flux

With interactions:





transport ~0

transport ≠ 0

$C \neq 0 \Leftrightarrow$ non-localized $w(\mathbf{r}) = \mathcal{F}[u(\mathbf{k})]$

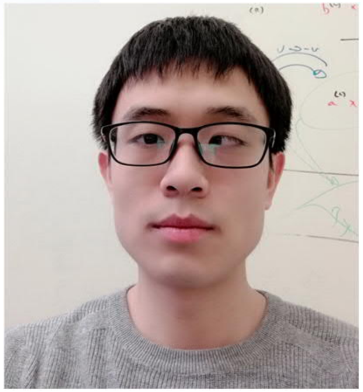
Brouder, Panati, Calandra, Marzari, PRL 2007

$$D_s \propto g_{ij} \geqslant C$$

Twisted bilayer graphene (TBG) superconductivity and quantum metric

Aleksi Julku

Teemu Peltonen



Long Liang

Tero Heikkilä

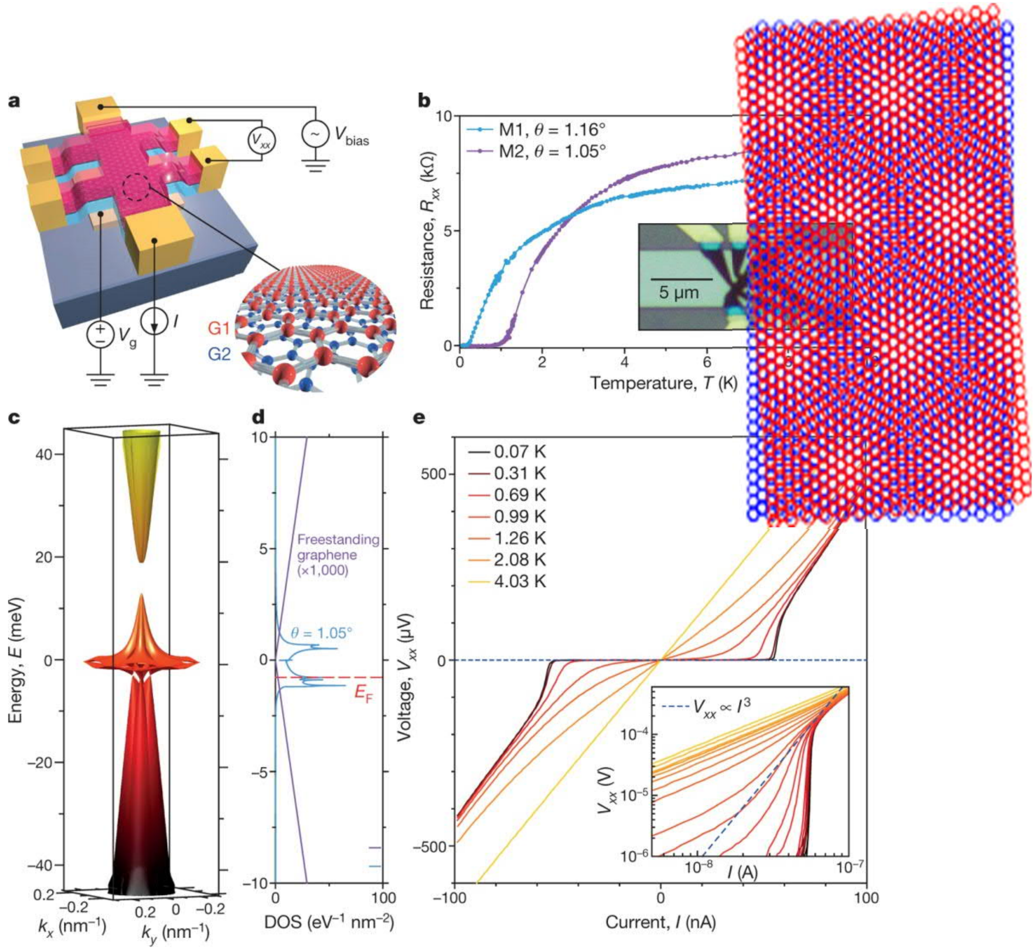
Julku, Peltonen, Liang, Heikkilä, PT, PRB(R) (2020); Editors' Suggestion

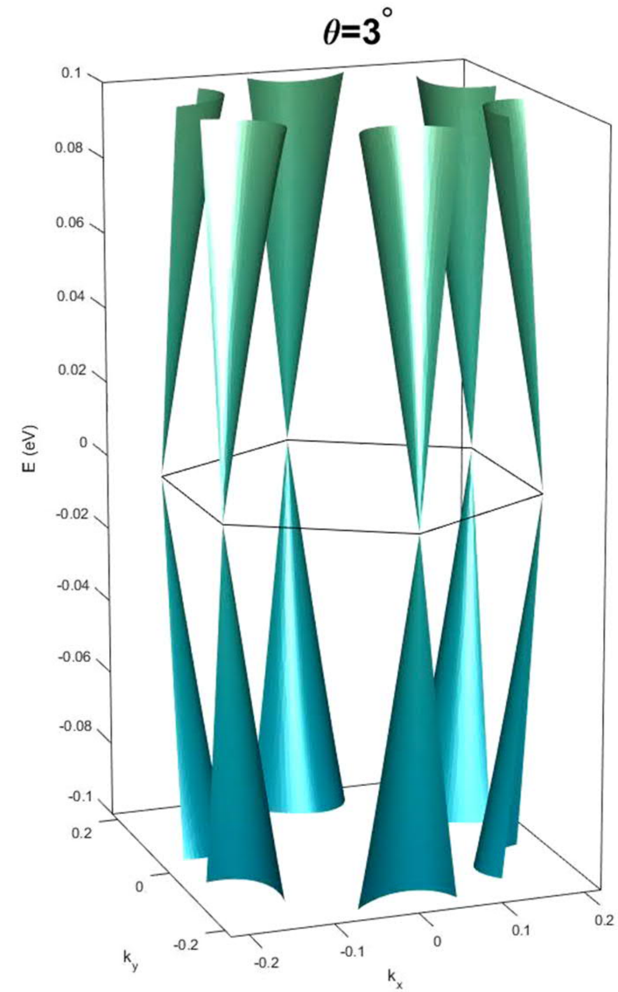
For APS Physics news, google Geometry resques superconductivity

MA-TBG: Magic **A**ngle**-T**wisted **B**ilayer **G**raphene

Twisting graphene layers produces flat bands

(unconventional) superconductivity





Y Cao *et al. Nature* **556**, 43–50 (2018)

Also

Nature 556, 80 (2018)

Science 363, 1059 (2019)

Nature 574, 653-657 (2019))

VIEWPOINT

PDF Version

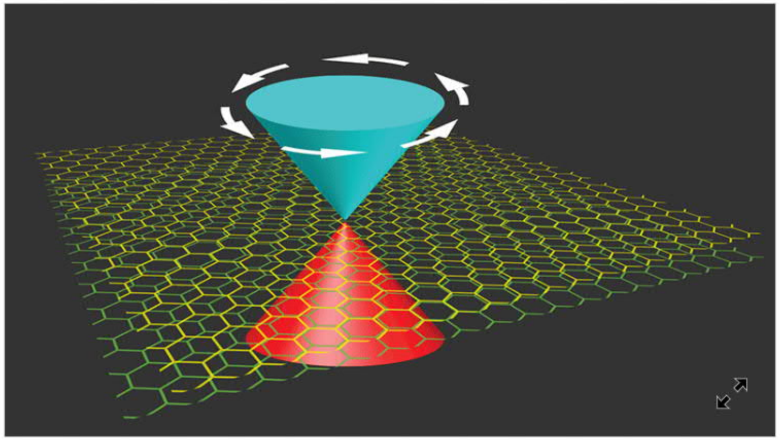
Geometry Rescues Superconductivity in Twisted Graphene

Laura Classen

School of Physics and Astronomy, University of Minnesota, Minneapolis, MN, USA

February 24, 2020 • *Physics* 13, 23

Three papers connect the superconducting transition temperature of a graphene-based material to the geometry of its electronic wave functions.



APS/Alan Stonebraker

Figure 1: Electrons moving through the sheets of twisted bilayer graphene (TBG) have special points in their band structure where two cone-shaped bands meet. The inherent "curvature" of the states in these bands turns out to contribute to the magnitude of TBG'... Show more

On its own, a sheet of graphene is a semimetal—its electrons interact only weakly with each other. But as experimentalists discovered in 2018 [1, 2], the situation changes when two sheets of graphene are stacked together, with a slight ($\sim 1^{\circ}$) rotation between them (Fig. 1). At this so-called magic twist angle [3] and at low temperatures [1], the electrons become correlated, forming insulating or superconducting phases depending on the carrier density [2–7]. These phases appear to come from a twist-induced flattening of the electronic energy bands, which

Geometric and Conventional Contribution to the Superfluid Weight in Twisted Bilayer Graphene

Xiang Hu, Timo Hyart, Dmitry I. Pikulin, and Enrico Rossi

Phys. Rev. Lett. 123, 237002 (2019)

Published December 5, 2019

Read PDF

Superfluid weight and Berezinskii-Kosterlitz-Thouless transition temperature of twisted bilayer graphene

A. Julku, T. J. Peltonen, L. Liang, T. T. Heikkilä, and P. Törmä

Phys. Rev. B 101, 060505 (2020)

Published February 24, 2020

Read PDF

Topology-Bounded Superfluid Weight in Twisted Bilayer Graphene

Fang Xie, Zhida Song, Biao Lian, and B. Andrei Bernevig

Phys. Rev. Lett. 124, 167002 (2020)

Published April 24, 2020

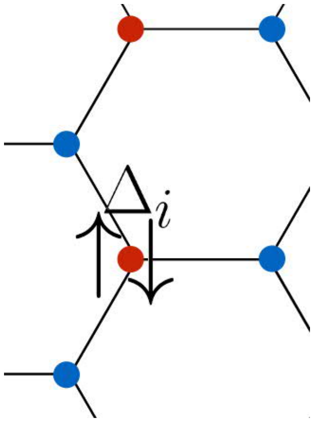
Read PDF

Fermi-Hubbard lattice model with TBG geometry:

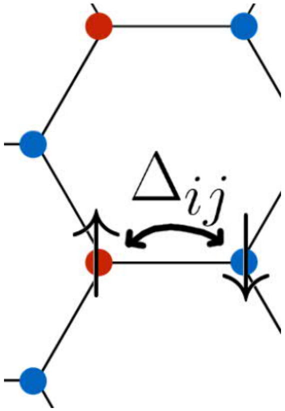
$$H = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + H_{\text{int}}$$

Two distinct pairing schemes:

$$H_{\text{int}} = J \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$



J< 0 is attractive interaction strength



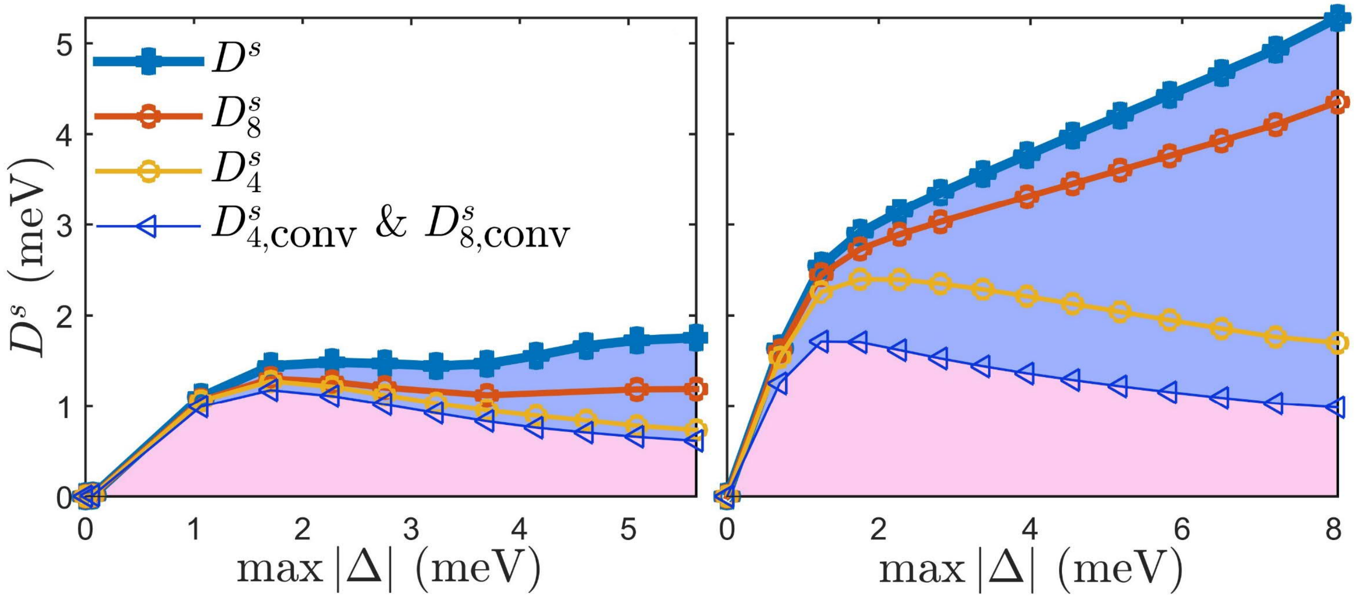
$$H_{\text{int}} = \frac{J}{2} \sum_{\langle ij \rangle} h^\dagger_{ij} h_{ij}$$

$$h_{ij} = c_{i\downarrow} c_{j\uparrow} - c_{i\uparrow} c_{j\downarrow}$$

Geometric contribution in TBG

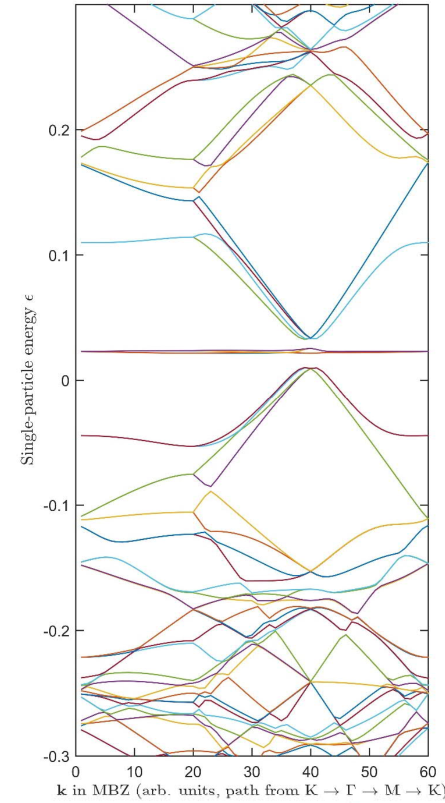
$$D^s = D^s_{\text{conv}} + D^s_{\text{geom}}$$

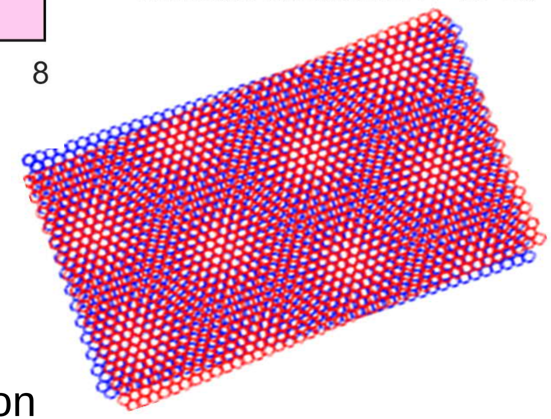
$$T_{\text{BKT}} = \frac{\pi}{8}\sqrt{\det D^s(T_{\text{BKT}})}$$



Non-local (RVB) interaction

Local (s-wave) interaction





Julku, Peltonen, Liang, Heikkilä, PT, PRB(R) (2020); Editors' Suggestion
Confirmed by (only s-wave): Hu, Hyart, Pikulin, Rossi, PRL (2019)
For APS Physics news, google Geometry resques superconductivity

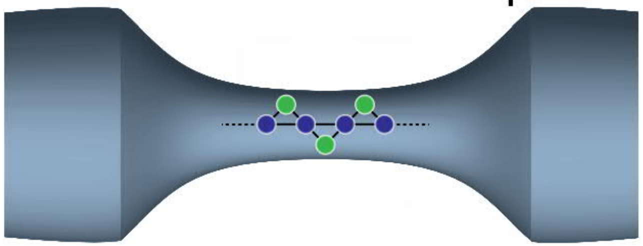
Flat band transport and Josephson effect through a saw-tooth lattice

Ville Pyykkönen Sebastiano Peotta Philipp Fabritius Jeffrey Mohan Tilman Esslinger

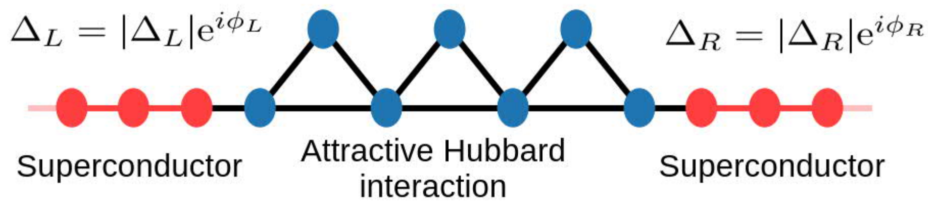
Pyykkönen, Peotta, Fabritius, Mohan, Esslinger, PT, PRB (2021)

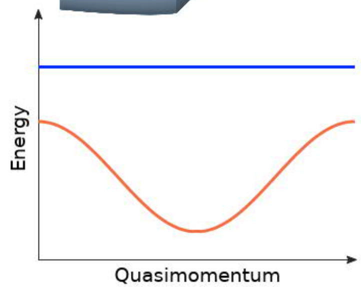
Ultracold sawtooth lattice transport setup

Two-terminal setup

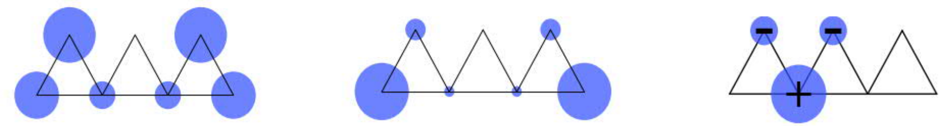


Tight-binding model





Truncation



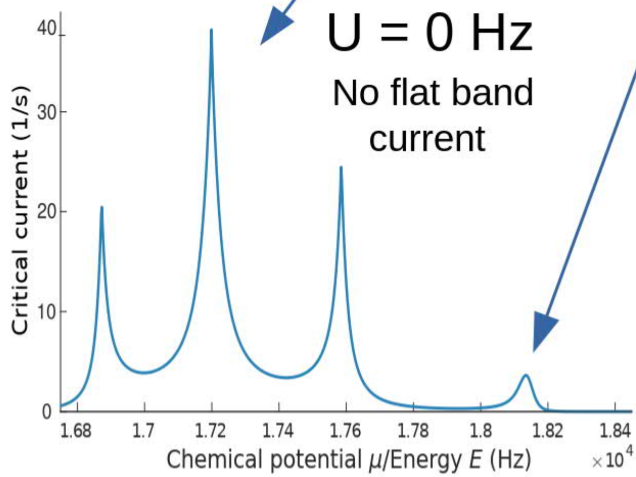
Dispersive band states

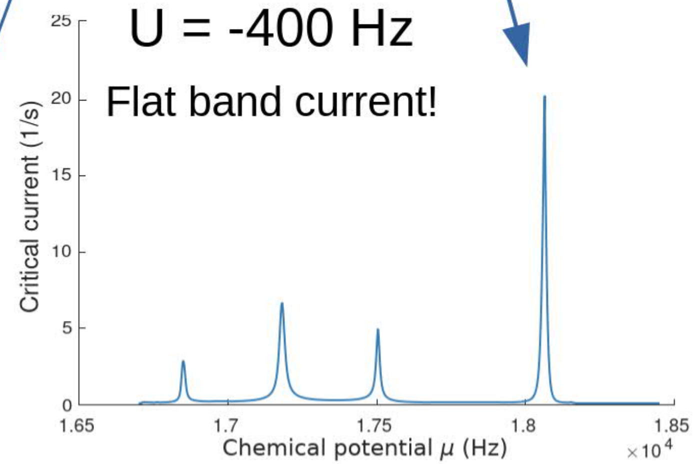
Edge states

Flat band states

Interaction → finite Josephson current through flat band states!

Optimal when edge and flat band states degenerate





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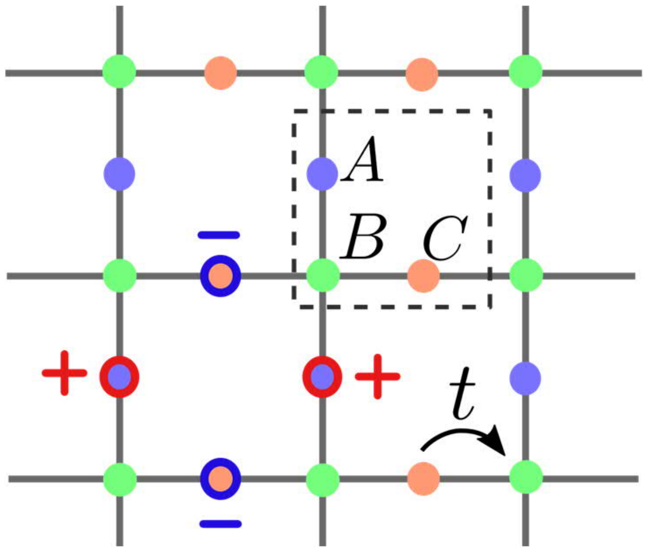
Pyykkönen, Peotta, Fabritius, Mohan, Esslinger and Törmä: Flat band transport and Josephson effect through a finite-size sawtooth lattice, PRB 103, 144519, 2021

Insulator – pseudogap crossover in the Lieb lattice normal state

Kukka-Emilia Huhtinen

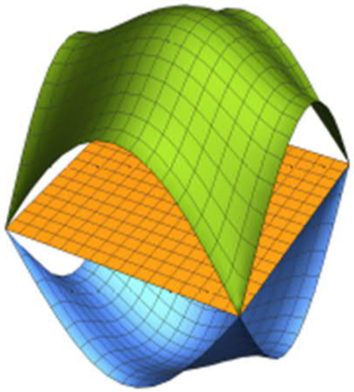
KE Huhtinen, PT, PRB(L) (2021)

Hubbard model on the Lieb lattice



Attractive Hubbard model

$$H = \sum_{\sigma} \sum_{i\alpha, j\beta} t_{ij} c^{\dagger}_{\sigma,i\alpha} c_{\sigma,j\beta} - \sum_{\sigma} \sum_{\mathrm{i}\alpha} \mu_\sigma n_{\sigma,i\alpha}$$
$$+U \sum_{i\alpha} (n_{\uparrow,i\alpha} - 1/2)(n_{\downarrow,i\alpha} - 1/2)$$

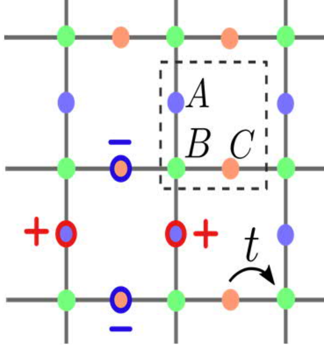


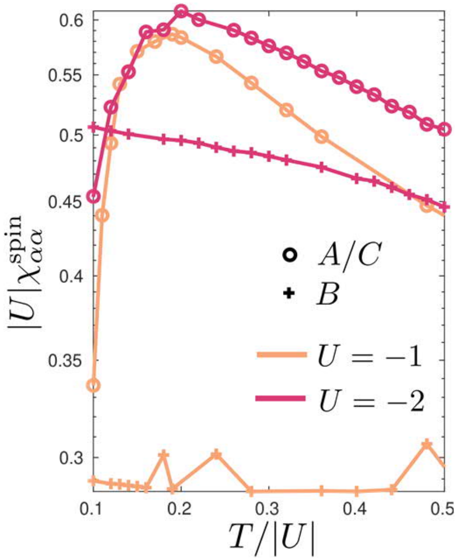
Flat band states reside at A and C sites

DMFT cluster: A, B and C

FOCUS ON THE NORMAL STATE ABOVE SUPERCONDUCTIVITY

Large (U>t) interactions: pseudogap





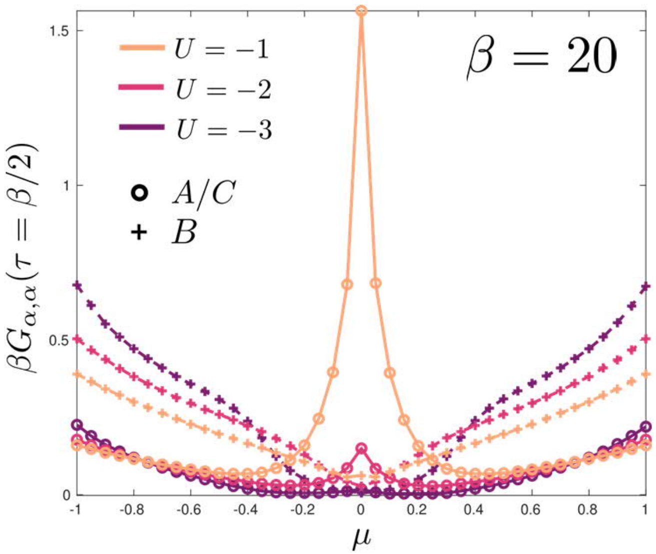
Generalized spin susceptibility:

$$\chi_{\alpha\alpha}^{\text{spin}} = \frac{2}{\beta^2}\sum_{\omega,\omega'}\left(\chi^{\text{ph},\omega,\omega',\nu=0}_{\uparrow\alpha,\uparrow\alpha,\uparrow\alpha,\uparrow\alpha} - \chi^{\text{ph},\omega,\omega',\nu=0}_{\uparrow\alpha,\uparrow\alpha,\downarrow\alpha,\downarrow\alpha}\right)$$

$$\chi_{ijkl}(\tau_1,\tau_2,\tau_3) = G^{(4)}_{ijkl}(\tau_1,\tau_2,\tau_3) - G_{ij}(\tau_1,\tau_2)G_{kl}(\tau_3,0)$$

$$G^{(4)}_{ijkl}(\tau_1,\tau_2,\tau_3) = \langle T_\tau[c_i^\dagger(\tau_1)c_j(\tau_2)c_k^\dagger(\tau_3)c_l(0)]\rangle$$

$$G_{ij}(\tau_1,\tau_2) = \langle T_\tau[c_i^\dagger(\tau_1)c_j(\tau_2)]\rangle$$

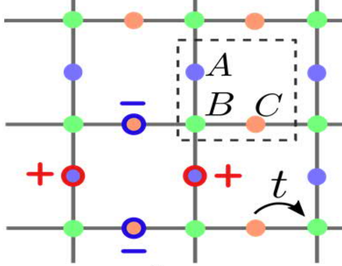


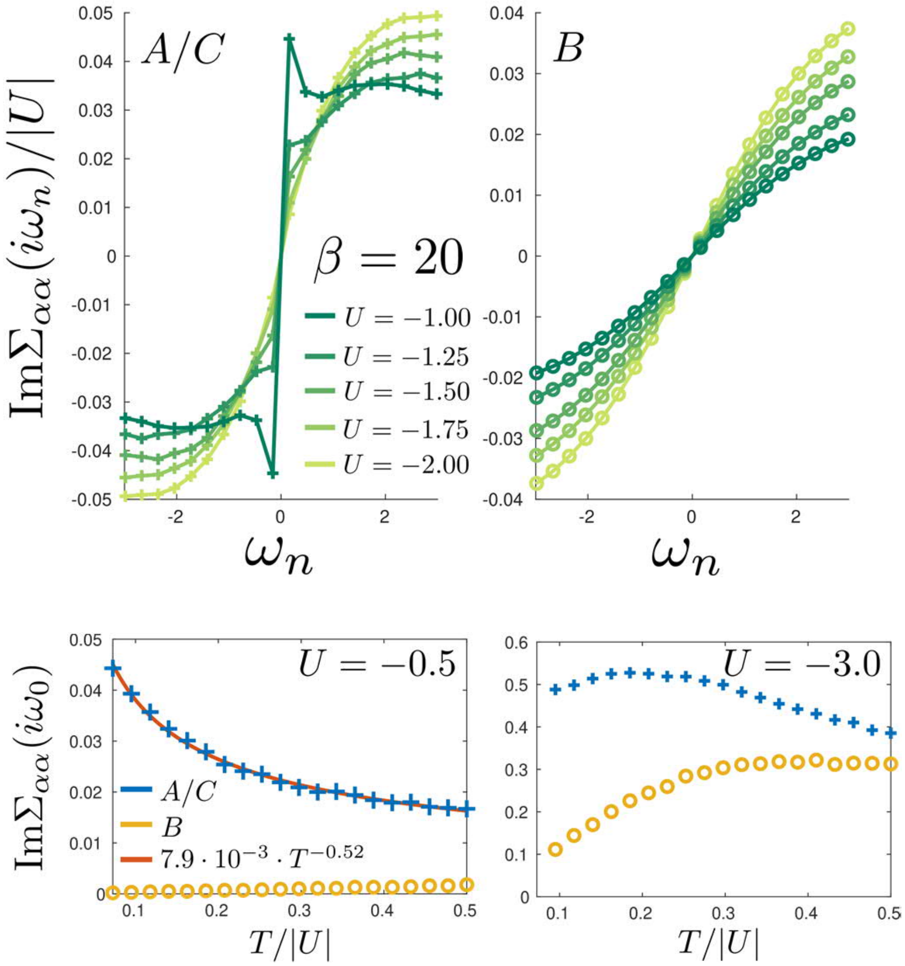
Local contribution to spin susceptibility decreases sharply with temperature at A/C sites.

At low temperatures, $\beta G_{\alpha\alpha}(\beta/2) \approx \mathcal{A}_\alpha(\omega=0)$, where $\mathcal{A}_\alpha$ is the orbital-resolved spectral function.

As interaction is increased, the spectral function becomes depleted around half-filling.

Low interaction (U<t): insulator





$$Z = \left(1 - \frac{\mathrm{Im}\Sigma(i\omega_n)}{\omega_n}\bigg|_{\omega_n \to 0}\right)^{-1}$$

In DMFT, $Z = m/m^*$, where m is the bare mass and m^* is the effective mass.

The self-energy diverges at low frequencies when the interaction strength is decreased.

The temperature dependence is $T^{-1/2}$ rather than T^{-1} found for Mott insulator.

Contents

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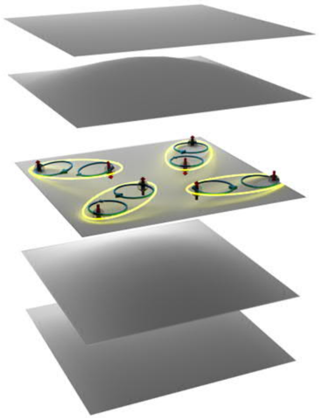
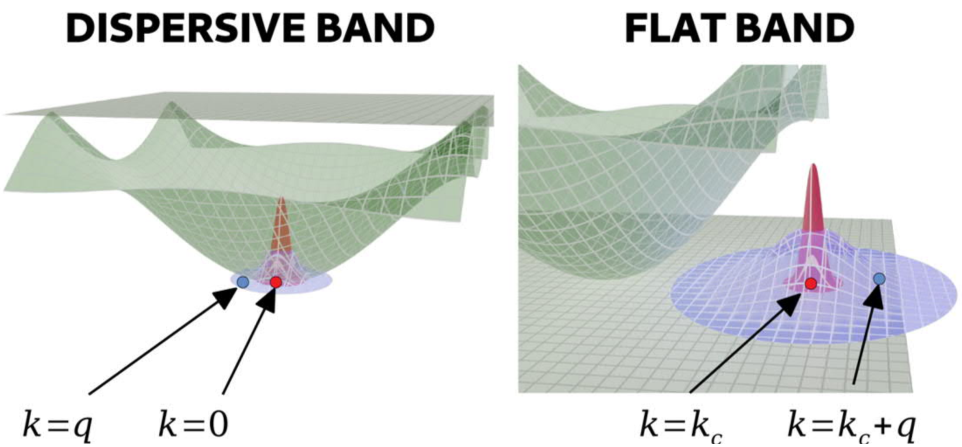
- What does quantum geometry have to do with this?

Quantum geometry and BEC

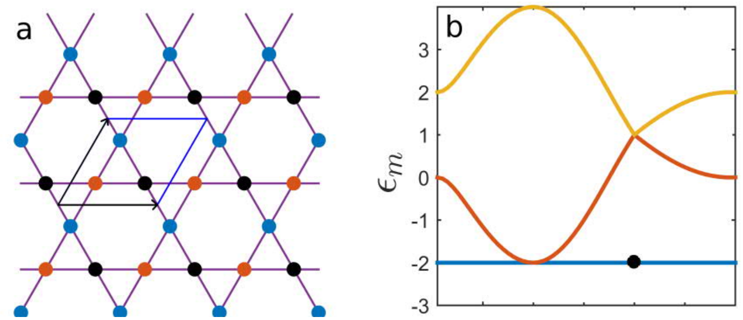
Quantum geometry and light-matter interactions



Flat band BEC & quantum geometry



Kagome lattice:

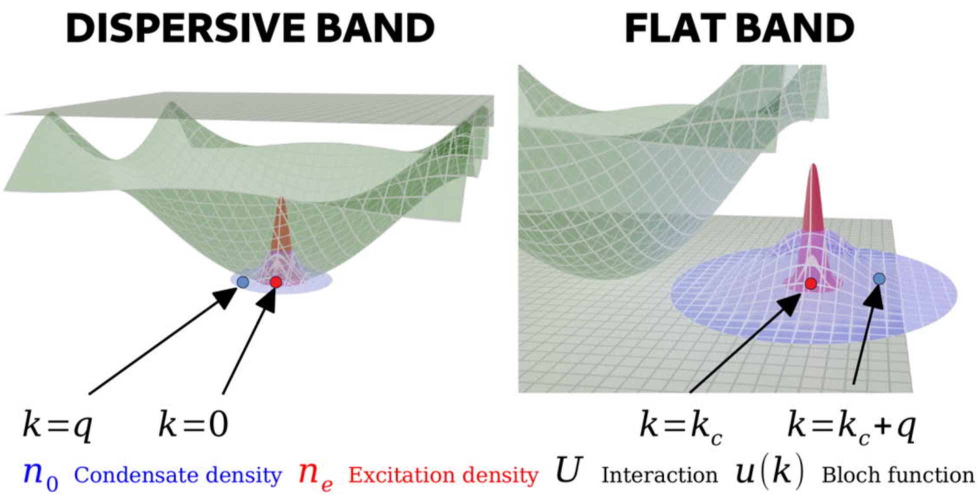


Aleksi Julku

Georg Bruun

Julku, Bruun, PT, arXiv:2104.14257

Flat band BEC & quantum geometry



SPEED OF SOUND

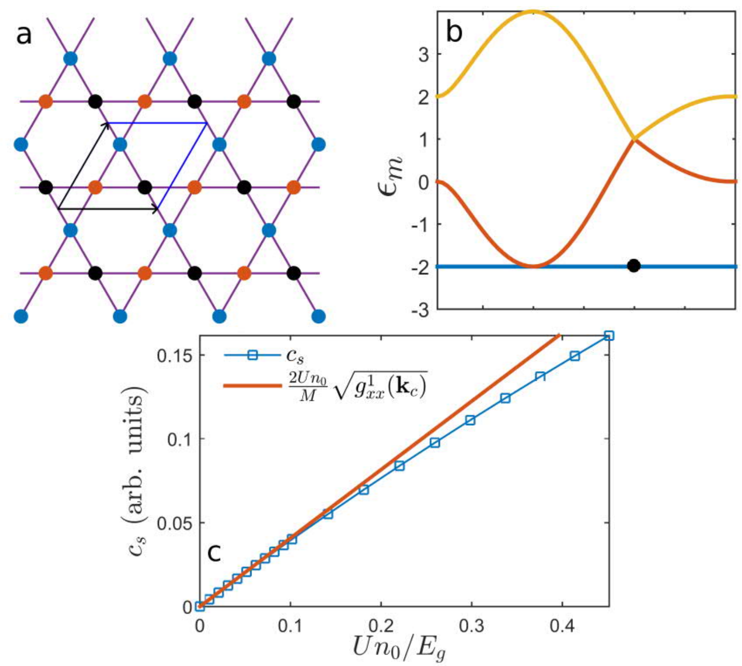
$$c_s \propto \sqrt{U n_0}$$

$$c_s \propto U n_0 \sqrt{g_{\alpha\beta}(k_c)}$$

Quantum metric

$$g_{\alpha\beta} = \Re[\langle \partial_\alpha u | \partial_\beta u \rangle - \langle \partial_\alpha u | u \rangle \langle u | \partial_\beta u \rangle]$$

Kagome lattice:



Quantum metric dictates the speed of sound

Aleksi Julku

Georg Bruun

Julku, Bruun, PT, arXiv:2104.14257

Flat band BEC & quantum geometry

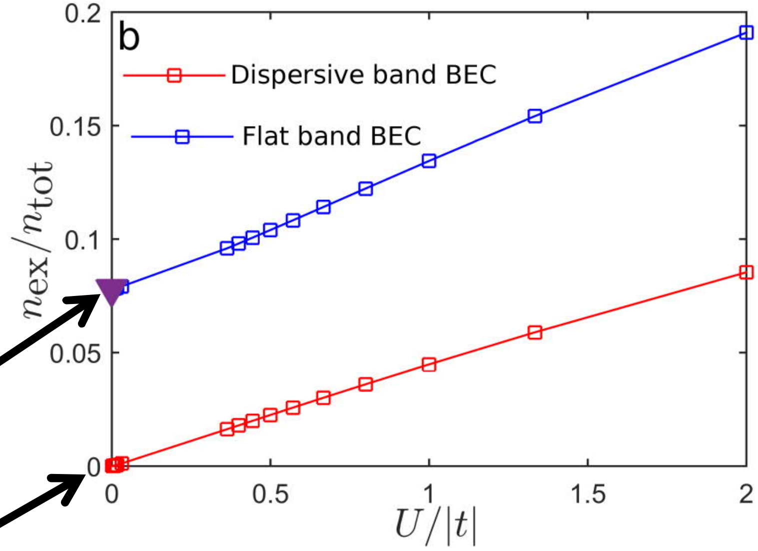
- Excitations do not cost energy? Can BEC stable?

Answer: Yes it can, finite **quantum distance** between Bloch states sets the limit for excitation density -> stable BEC

$$n_e(k) \xrightarrow[U\to 0]{} \frac{1-D}{2D}$$

Quantum distance

$$D = \sqrt{1 - |\langle u(k_c+q) | u(k_c-q)\rangle|^2}$$



Excitation density can be finite in the non-interacting limit...

...in contrast to dispersive band BEC

Interaction effects prominent even in the limit of vanishing interactions

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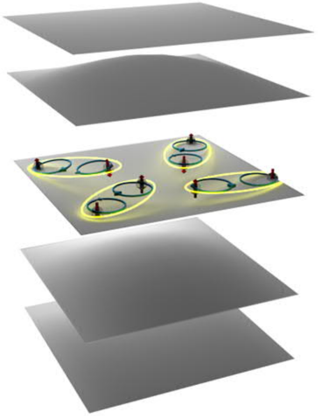
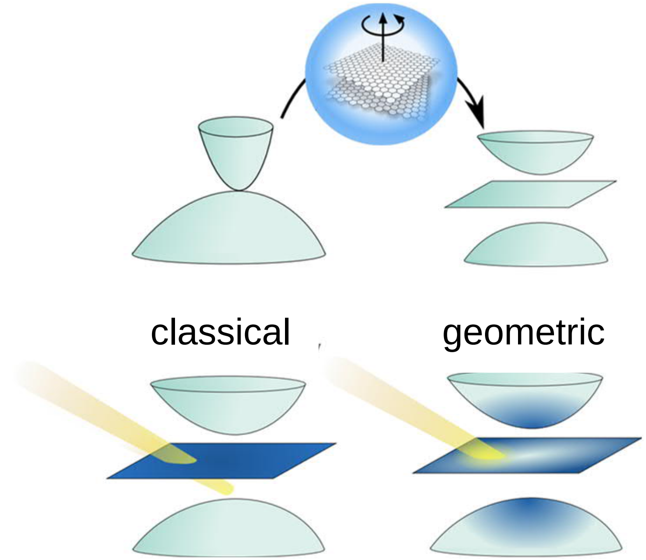


Light-matter coupling (LMC) in multi-band systems



G. E. Topp, C. J. Eckhardt, D. M. Kennes, M. A. Sentef, and PT, PRB 2021

Reminder: Single-band LMC

$$H_{\mathrm{LMC}}^{\mathrm{single}} = \sum_{\mu} \partial_{k\mu}\epsilon(k)\cdot A_\mu + \frac{1}{2}\sum_{\mu\nu}\partial_{k\mu}\partial_{k\nu}\epsilon(k)\cdot A_\mu A_\nu$$

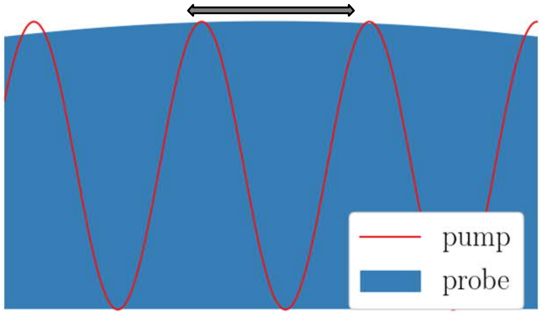
paramagnetic diamagnetic

	Linear (A_μ)	**Quadratic** $(A_\mu A_\nu)$
Intra-band (n)	$\boxed{\partial_\mu \varepsilon_n}$	$\boxed{\partial_\mu\partial_\nu\varepsilon_n} - \boxed{\sum_{n\neq n'}(\varepsilon_n - \varepsilon_{n'})\left(\langle\partial_\mu n\,\|n'\rangle\langle n'\,\|\partial_\nu n\rangle + \mathrm{h.c.}\right)}$
Inter-band $(n,\, m)$	$\boxed{(\varepsilon_n - \varepsilon_m)\langle m\,\|\partial_\mu n\rangle}$	$\boxed{\Big[(\partial_\mu\varepsilon_n - \partial_\mu\varepsilon_m)\langle m\,\|\partial_\nu n\rangle + \frac{1}{2}\varepsilon_m\langle\partial_\mu\partial_\nu m\,\|n\rangle + \frac{1}{2}\varepsilon_n\langle m\,\|\partial_\mu\partial_\nu n\rangle + \sum_{n'}\varepsilon_{n'}\left(\langle\partial_\mu m\,\|n'\rangle\langle n'\,\|\partial_\nu n\rangle\right)\Big] + (\mu\leftrightarrow\nu)}$

- ‘classical’ = determined by band dispersion
- ‘geometric’ = determined by Bloch states

Floquet theory

$$\Omega = \frac{2\pi}{T}$$



$$H(t)\psi - \mathrm{i}\partial_t \psi = 0$$

$$H(t) = H(t+T)$$

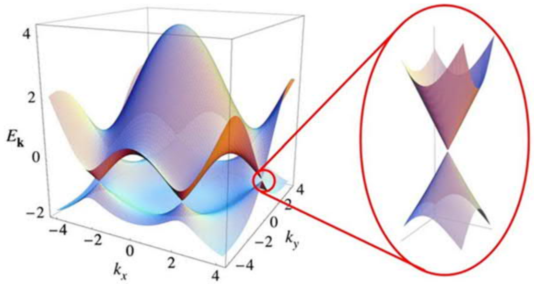
$$\Psi(t) = e^{-\mathrm{i}\epsilon t} \sum_{m=-\infty}^{\infty} \phi_m e^{-\mathrm{i}m\Omega t}$$

$$\sum_{m=-\infty}^{\infty} \mathcal{H}^{mn} \phi_\alpha^m = \epsilon_\alpha \phi_\alpha^n$$

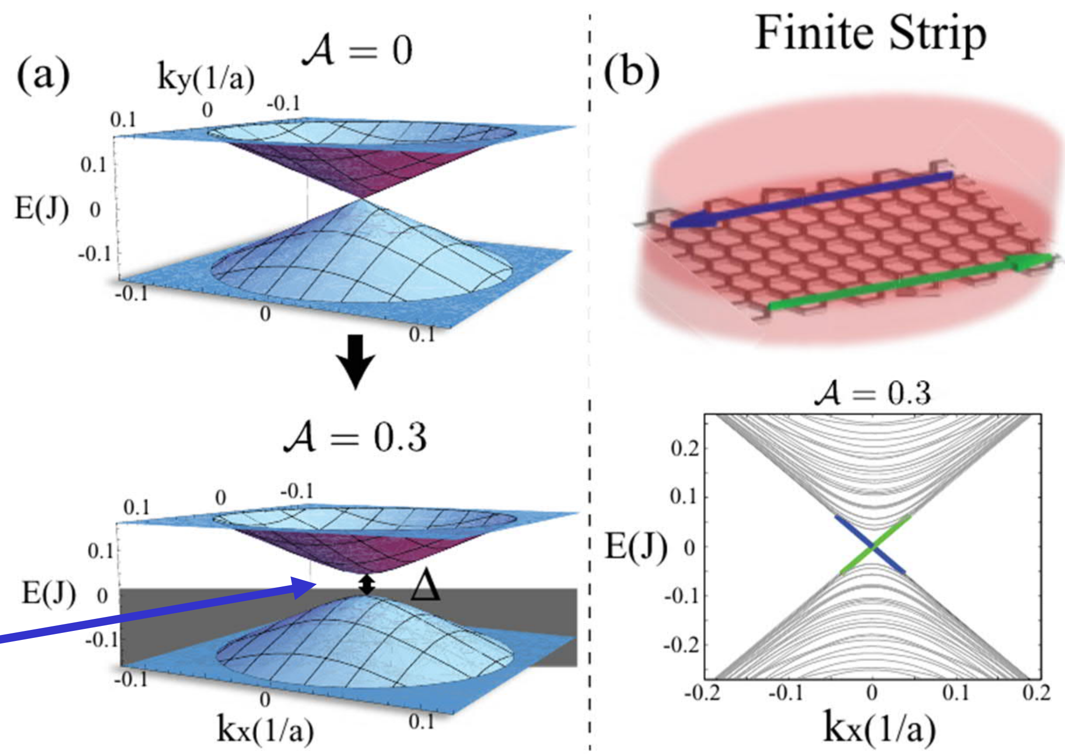
Floquet Hamiltonian:

$$\mathcal{H}^{mn} = \frac{1}{T} \int_0^T \mathrm{d}t H(t) e^{\mathrm{i}(m-n)\Omega t} + m\delta_{mn}\Omega t$$

QAHE in graphene



Neto, et al., Rev. Mod. Phys. 81 (2009)



circular drive:

$$H_{\text{eff}} \approx H_0 + \frac{[H_{-1}, H_1]}{\Omega} + O(\mathcal{A}^4)$$

$$\approx v_G(\sigma_y k_x - \sigma_x k_y \tau_z) \boxed{\pm \frac{v_G^2 \mathcal{A}^2}{\Omega} \sigma_z \tau_z} + O(\mathcal{A}^4)$$

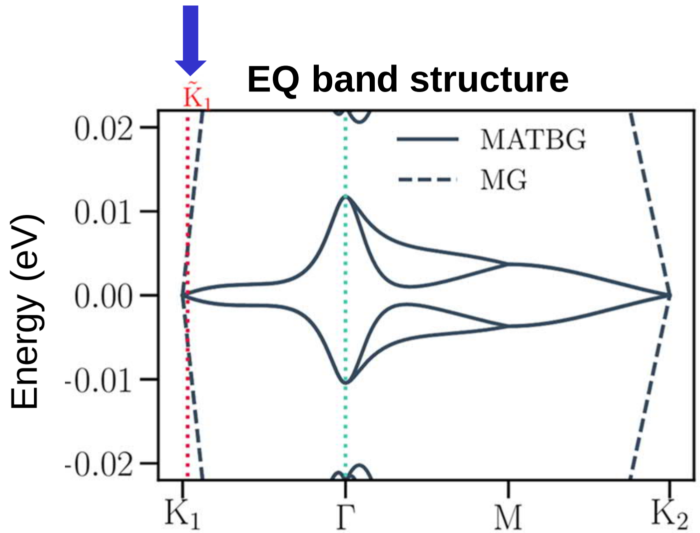
breaks TRS

T. Oka & H. Aoki, PRB 79, 081406 (2009)
Kitagawa et al. PRB 84, 235108 (2011)

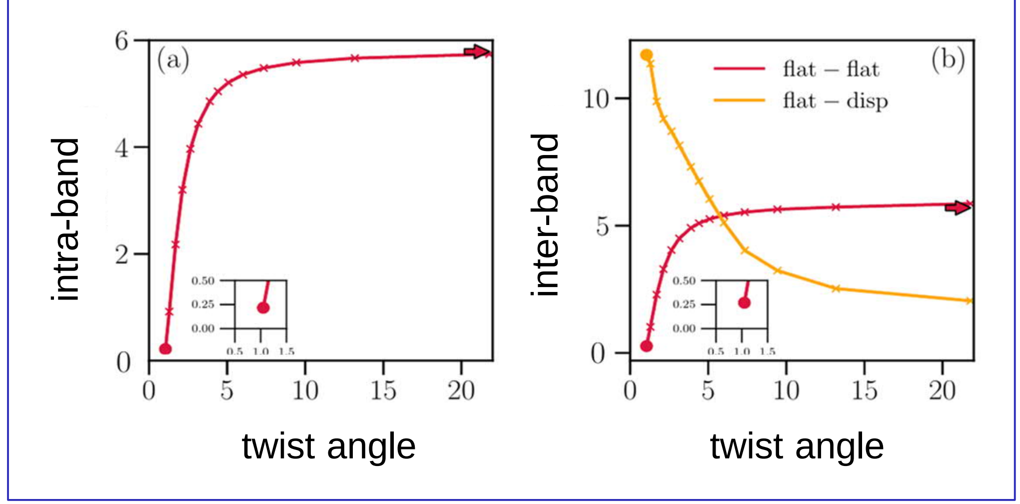
Application: Light-induced Dirac gap in TBG

G. E. Topp, C. J. Eckhardt, D. M. Kennes, M. A. Sentef, and PT, PRB 2021

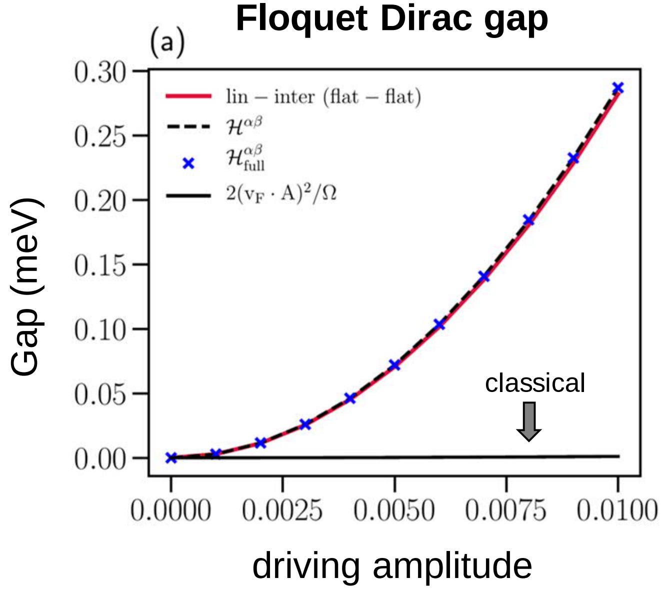
EQ band structure

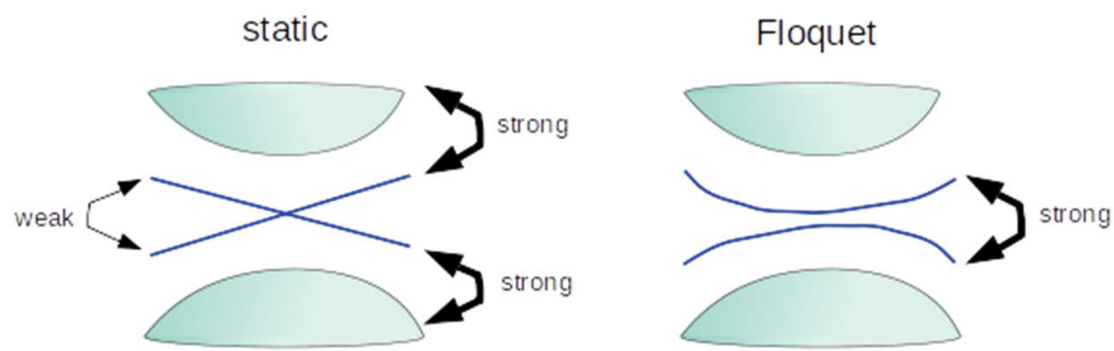


Linear LMC



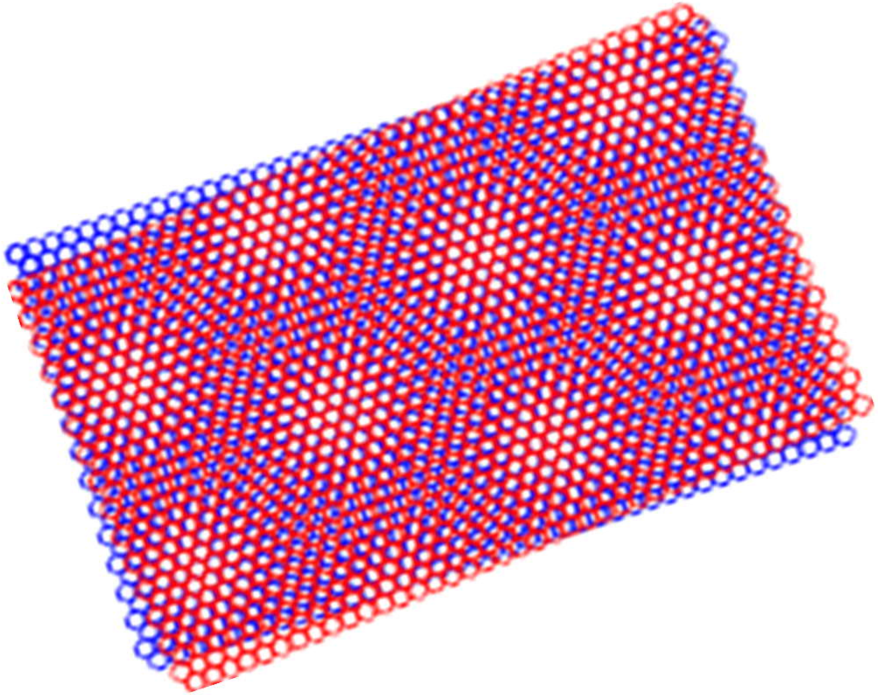
Floquet Dirac gap





$$\langle m | H^A_{\mathrm{FLOQ}} | n \rangle = \frac{\mathrm{i} A_0^2}{2\Omega} \left[\sum_l \langle m | \frac{\partial H_0}{\partial k_x} | l \rangle \langle l | \frac{\partial H_0}{\partial k_y} | n \rangle - \langle m | \frac{\partial H_0}{\partial k_y} | l \rangle \langle l | \frac{\partial H_0}{\partial k_x} | n \rangle \right]$$

Summary



Quantum geometry governs
- flat band superfluidity
- BEC excitations
- light-matter interactions

Outlook

Towards room temperature superconductivity

Role of quantum geometry and interactions
in photonic systems

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