Title: A triangular-lattice spin-valley Hubbard model in the ABC trilayer graphene/h-BN moire system

Date: Oct 30, 2018 03:30 PM

URL: http://pirsa.org/18100044

Abstract: <p>This year there appear several amazing experiments in the graphene moire superlattices. In this talk I will focus on the ABC trilayer graphene/h-BN system. Mott-like insulators at 1/4 and 1/2 of the valence band have already been reported by Feng Wangâ€™s group at Berkeley. The sample is dual gated on top and bottom with voltage V_t and V_b. V_t+V_b controls the density of electrons. Interestingly we find that the displacement field D=V_t-V_b can control both the topology and the bandwidth of the valence band. For one sign of D (for example D>0), there are two narrow Chern bands with opposite Chern numbers C=3,-3 for the two valleys. For D<0, the bands of the two valleys are trivial and have localized Wannier orbitals on a triangular lattice. As a result, the physics is governed by a spin-valley Hubbard model on a triangular lattice. This talk focuses on the D<0 side and consists of two parts: (1) I will provide the details of this spin-valley Hubbard model and discuss some subtleties special to the moire systems.   (2) In the second part I want to show some of our theoretical attempts on this Hubbard model. First I will show that this system is a perfect platform for studying metal-insulating transition. I will provide a theory of continuous Mott transition between a Fermi liquid and a spinon Fermi surface Mott insulator. Second I will discuss some possible metallic phases upon doping away from the Mott insulator. Unlike the familiar spin 1/2 case, the spin-valley Hubbard model may not be in a conventional Fermi liquid phase even in the over-doped region. I will provide some candidates of possible unconventional metals based on a six-flavor slave boson theory for the hole doped side.</p>

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<p>References:</p>

<p>Feng Wang et.al. arxiv: 1803.01985</p>

<p>Ya-Hui Zhang, Dan Mao, Yuan Cao, Pablo Jarillo-Herrero and T. Senthil. arXiv:1805.08232</p>

<p>Ya-Hui Zhang and T. Senthil, arxiv: 1809.05110</p>

<p>Ya-Hui Zhang and T. Senthil, ongoing work</p>

Bridging Hubbard Model Physics and Quantum Hall Physics in trilayer Graphene moire superlattice

Ya-Hui Zhang
(MIT)

References:

Y-H. Zhang, D. Mao, C. Yuan, P. Jarillo-Herrero, T. Senthil arxiv:1805.08232

Y-H. Zhang and T. Senthil, arxiv: 1809.05110

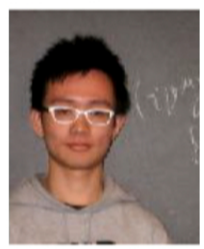
Collaborators at MIT

T. Senthil

Cécile Repellin

Collaborators in Bilayer Graphene/ Bilayer Graphene System:

Dan Mao

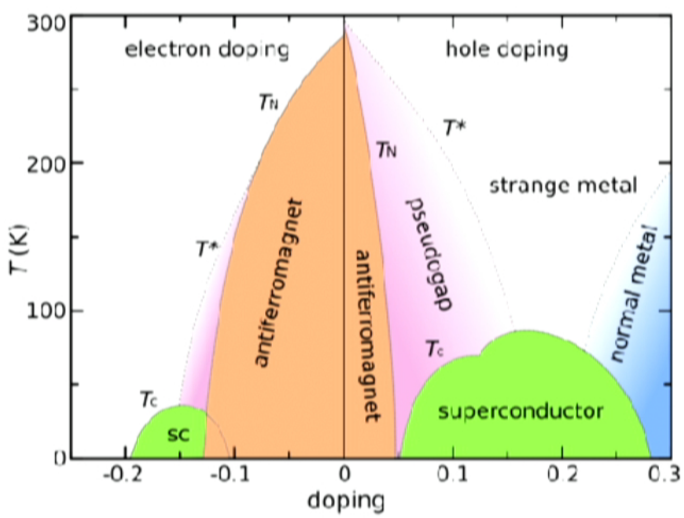


Yuan Cao

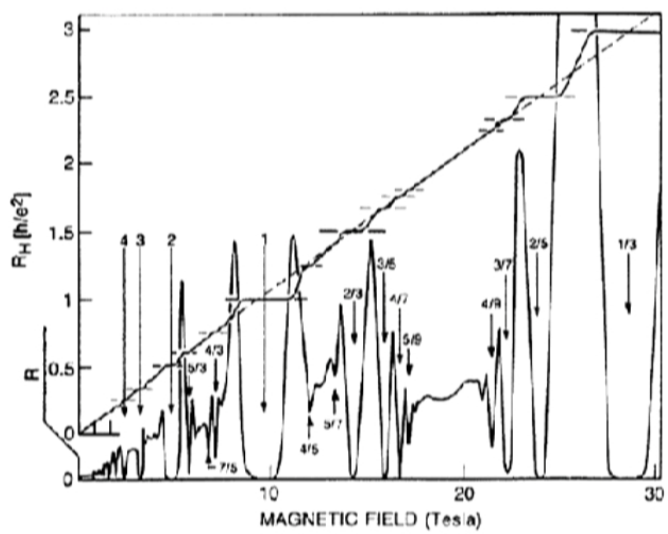
Pablo Jarillo-Herrero

Motivation: Cuprate and Quantum Hall System

30 years old problems:



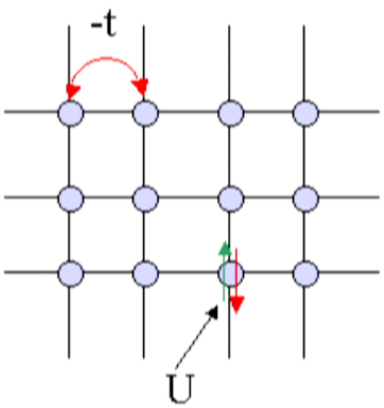
Cuprate



Quantum Hall

Cuprate

Square Lattice Hubbard Model



Exotic Phases:

high-Tc superconductor

pseudogap metal

strange metal

No theoretical agreement.

Is the physics governed by doped Mott Insulator ?

Are these phases universal to Hubbard model?

We need other realizations of doped Mott insulator.

Quantum Hall states

Theory is well established.

Need more experimental controls of anyons.

Can we trap anyon inside a vortex in a quantum Hall/ SC heterostructure?

Is FQHE at zero magnetic field possible?

Narrow Chern Band

Gate tunable density.

Need Strongly Correlated Systems with high Controllability

Hard in conventional solid-state material.

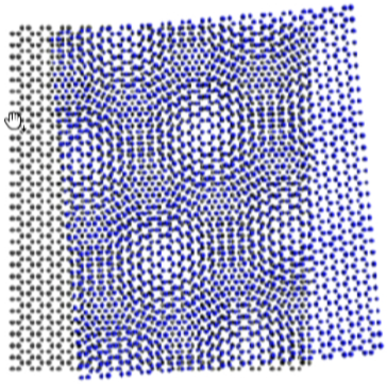
Cold atom: Temperature is too high (1000K now!)

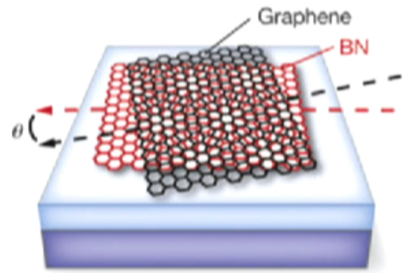
Moire Superlattice is a perfect platform!

Bandwidth and Interaction: 100K.

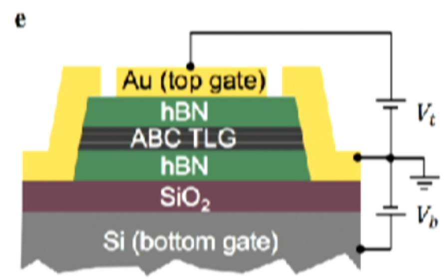
Experiment regime: 100 mK; Low enough for superconductor.

ABC Trilayer Graphene on Hexagonal Boron Nitride





Feng Wang et.al. arxiv:1803.0198



D: a vertical electric field

Switch between two different physics:

Triangular Lattice Hubbard Model ⟷ **Nearly Flat** $C = \pm 3$ **Chern Bands**

D<0

D>0

"Cuprate" Physics

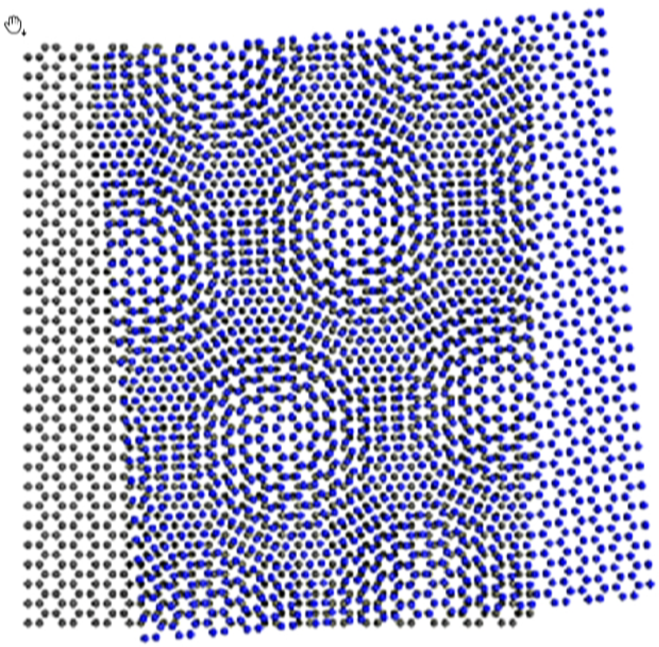
"Quantum Hall" Physics

Y-H. Zhang and T. Senthil, arxiv: 1809.05110

Y-H. Zhang, et.al and T. Senthil, arxiv:1805.08232

Moire Superlattices

Explored for one decade



$$|e^{iG_1x} + e^{iG_2x}|^2 \sim e^{i(G_1-G_2)x} + \ldots$$

Moire reciprocal vector: $\vec{G}_M = \vec{G}_1 - \vec{G}_2$

Almost identical lattice constant:

$$|G_1| \approx |G_2| \approx |G_0|$$

θ : twisted angle

$$\epsilon = \frac{||G_1| - |G_2||}{|G_0|} = \frac{|a_1 - a_2|}{a_0}$$

$$G_M \sim \sqrt{\epsilon^2 + \theta^2} G_0 << G_0$$

Typical value: $a_M \sim 60 a_0 \sim 15$ nm

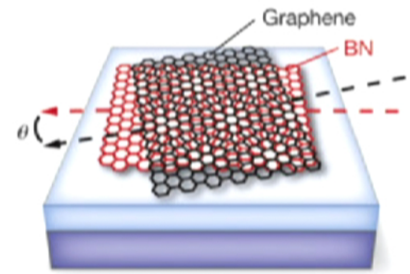
Strongly correlated effects from moire superlattice: band folding!

Bandwidth decreases faster than interaction $U \sim 1/a_M$

Graphene aligned with Hexagonal Boron Nitride

h-BN: band gap at order eV

$$G_M \sim \sqrt{\epsilon^2 + \theta^2} G_0$$

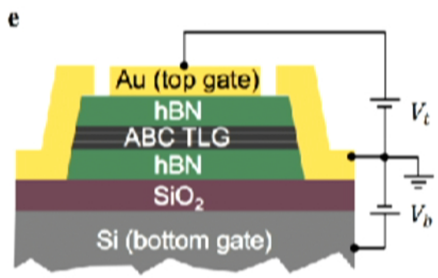


Zero twist angle:

$$\epsilon = \frac{a_1 - a_2}{a_1} = 1.7\% \qquad a_M \approx 58a \text{ around 15 nm.}$$

ABC Trilayer Graphene/h-BN (TG/h-BN):

$\theta_1 = 0$ $\qquad$ θ_2 very large



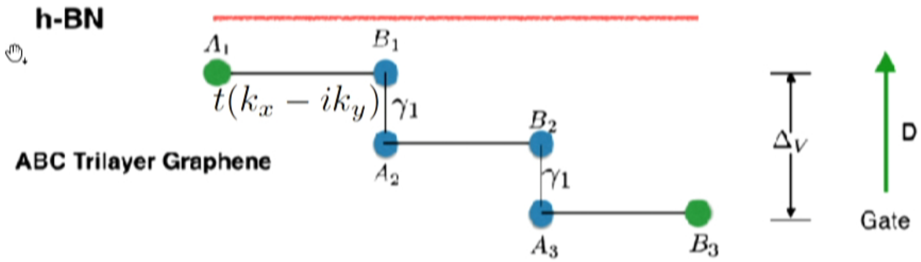
Effects of h-BN:

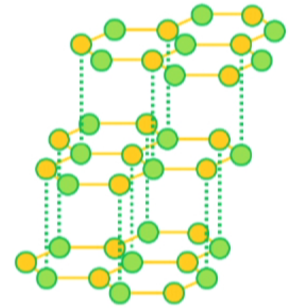
super-lattice potential for electrons in graphene.

Strongly correlated effects emerge!

Feng Wang et.al. arxiv:1803.0198

Model Single ABC Trilayer Graphene





$\gamma_1 \approx 400$ meV. Relevant Energy scale in this talk: 30 meV.

Two valleys at K and K'. Three Dirac cones in the decoupling limit.

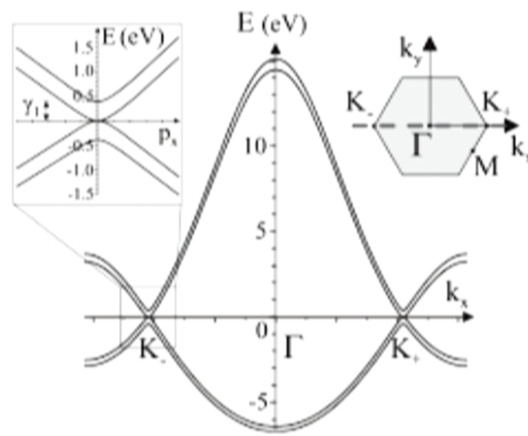
At neutrality, only two bands at low energy:

$$h_+(\mathbf{k}) = \begin{pmatrix} \frac{\Delta_V}{2} & \frac{t^3}{\gamma_1^2}(k_x - ik_y)^3 + 2\frac{t\gamma_3}{\gamma_1}|\mathbf{k}|^2) \\ \frac{t^3}{\gamma_1^2}(k_x + ik_y)^3 + 2\frac{t\gamma_3}{\gamma_1}|\mathbf{k}|^2) & -\frac{\Delta_V}{2} \end{pmatrix}$$

$\psi = (c_{A_1}, c_{B_n})$ Δ_V: Voltage between top and bottom

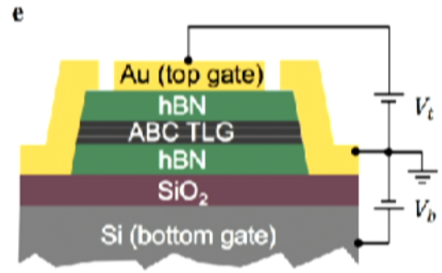
Time reversal: $h_-(\mathbf{k}) = h_+^*(-\mathbf{k})$

Mass term of the cubic touching is gate tunable!



A.H. MacDonald, arxiv: 0806. 2792

Moire Superlattice Potential

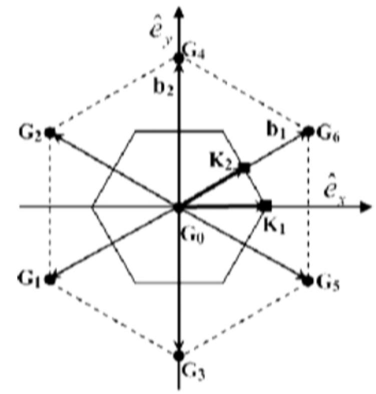


For one valley:

$$H_M = \sum_{\mathbf{G_j}} \sum_{\mathbf{k}} \psi^\dagger(\mathbf{k} + \mathbf{G}_j) \begin{pmatrix} V_0 e^{i\theta_j} & 0 \\ 0 & 0 \end{pmatrix} \psi(\mathbf{k}) + h.c.$$

DFT estimation: $V_0 \sim 10meV$ Jeil Jung, et.al. , A.H. Macdonald, Phys. Rev . B 89, 205414 (2014)

Free Electron Approximation.



G_j : Reciprocal vector of a Hexagon Moire Brillouin Zone (MBZ)

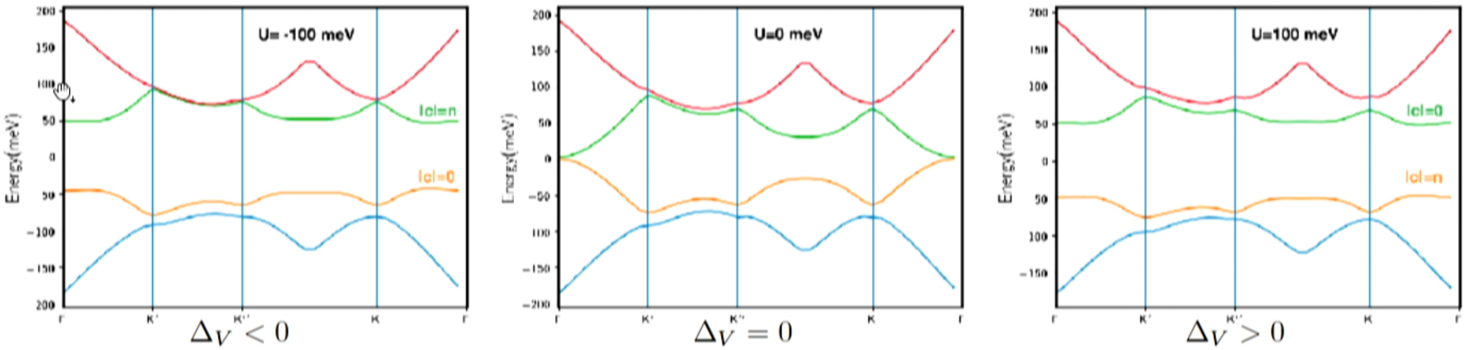
No valley scattering: $|G_j| = |G_M| << |K - K'|$

We move band crossing point of two valleys to Γ point of MBZ.

$$|G_M| \sim \frac{1}{60} |G_{original}|$$

Valley can be viewed as a pseudo-spin.

Bilayer Graphene/h-BN band dispersion for one valley:



Trilayer Graphene/h-BN is similar.

Y-H. Zhang, et.al and T. Senthil, arxiv:1805.08232

Higher Angular-Momentum Band Inversion:

For valley +: $C(\Delta_V > 0) - C(\Delta_V < 0) = n$

For TG/h-BN:

$\Delta_V > 0$ Narrow C=$\pm$3 Chern Bands

$\Delta_V < 0$ Narrow Trivial Bands

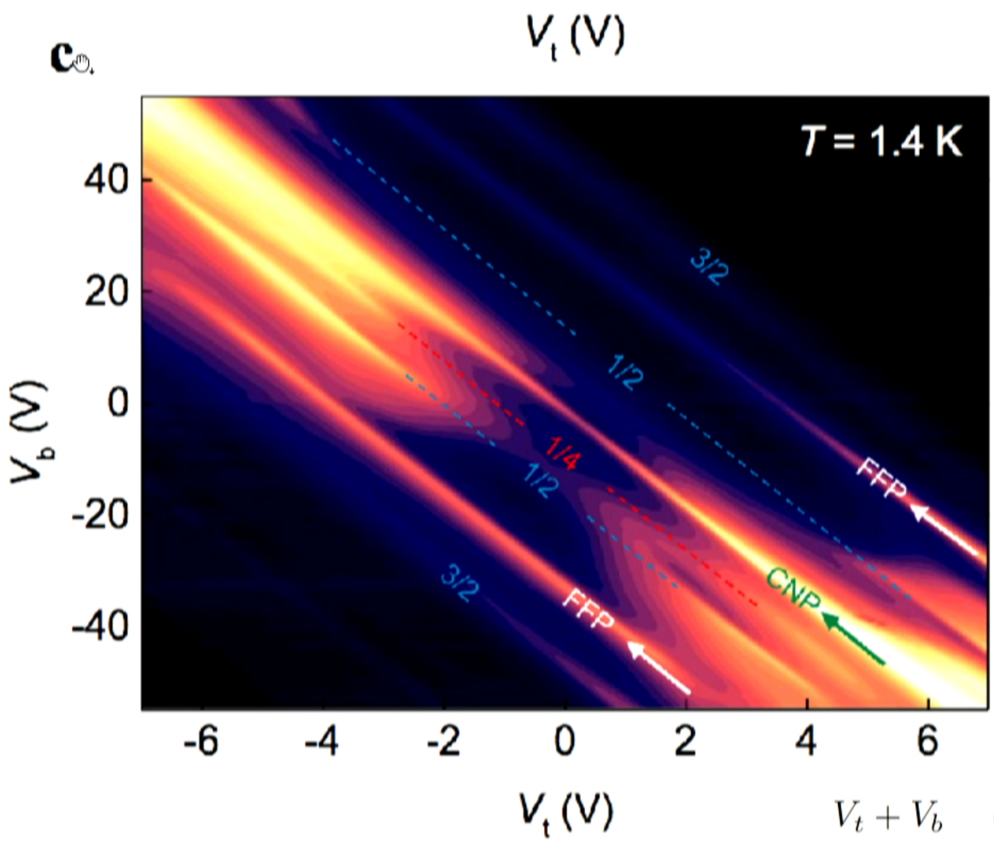
$$h_+(\mathbf{k}) = \begin{pmatrix} \frac{\Delta_V}{2} & \frac{t^3}{\gamma_1^2}(k_x - ik_y)^3 + 2\frac{t\gamma_3}{\gamma_1}|\mathbf{k}|^2) \\ \frac{t^3}{\gamma_1^2}(k_x + ik_y)^3 + 2\frac{t\gamma_3}{\gamma_1}|\mathbf{k}|^2) & -\frac{\Delta_V}{2} \end{pmatrix}$$

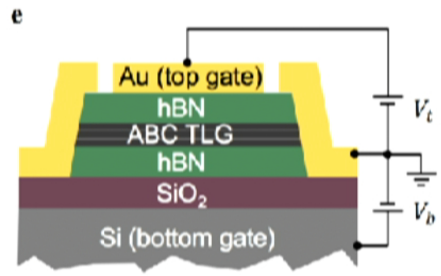
We focus on the valence band: four species + up, + down, - up, -down.

Experimental Results for TG/h-BN

Correlated Insulators has been found at $\nu_T = 1, 2$

Feng Wang et.al. arxiv:1803.0198





Valence band: four bands; spin, valley

number of holes per unit cell

$\nu_T = 4\nu$

Color map: Resistance

$V_t + V_b$ **Controls the filling.**

$\Delta_V = V_t - V_b$ **Controls the bandwidth and topology.**

The other system: twisted bilayer graphene

Monolayer graphene on monolayer graphene

Correlated insulator and superconductor

Cao, Fatemi et al, Nature **556**, 80 (2018)
Cao, Fatemi et al, Nature **556**, 43 (2018)

However, no simple lattice model so far!

Yankowitz, Chen et.al. arxiv: 1808. 07865

A simple Hubbard model seems not very likely.

Advantage of TG/h-BN

Gate Tunable Bandwidth and Topology

One band per spin valley

Simple model

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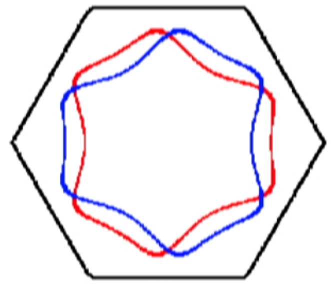
Simple model

Symmetry

Four Flavors of valence band: + up, + down, - up, - down.



Both kinetic term and interaction break U(4).

Density Operator:

$$\rho_{a,\sigma}(\mathbf{q}) = \sum_{\mathbf{k}} \lambda_a(\mathbf{k}, \mathbf{k}+\mathbf{q}) c^\dagger_{a,\sigma}(P(\mathbf{k}+\mathbf{q})) c_{a,\sigma}(\mathbf{k}) + \ldots$$

Form factor: contains information of Berry connection.

Approximating Symmetry: $U(2)_+ \times U(2)_- \times T$

$c^\dagger_+ c_- V(2K) c^\dagger_- c_+$ leads to: $-J_H \mathbf{S}_+ \cdot \mathbf{S}_-$

Good Symmetry: $U(1)_c \times U(1)_v \times SU(2)_s \times T$

Next Part

I. Trivial Side: Spin-Valley Hubbard Model

(1) Spin model for the strong Mott insulators.

(2) Metal-Insulator Transition

II. Chern Side: C=3,-3 Narrow Bands

(1) Flat band limit: Chern Insulator with $\sigma_{xy} = 3\frac{e^2}{h}$

(2) Fractional Filling at Flat Band limit

Trivial Side

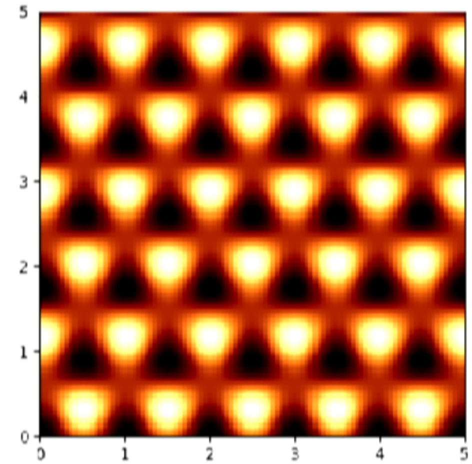
Wannier Orbital

- Bright points form Triangular Lattice.

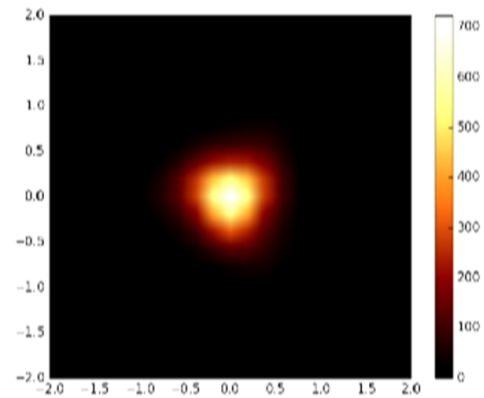
Each valley: Wannier orbital at bright point.

$$|w(\mathbf{x_0})\rangle = \frac{1}{\sqrt{N}} \sum_k e^{i\theta(\mathbf{k})} c_k^\dagger |0\rangle$$

Projection methods to choose $\theta(\mathbf{k})$



Density of valence band.



Wannier Orbital

Trivial Side

Lattice Model

Spin-Valley Hubbard Model on Triangular Lattice:

$$H = H_t + H_U + \ldots$$

Building block: $c_{i;a\sigma}$

H_U : on-site Hubbard U

a=+,- valley index

$\sigma = \uparrow, \downarrow$ spin index

… terms:

on-site Inter-valley Hund's $-J_H \mathbf{S}_+ \cdot \mathbf{S}_-$

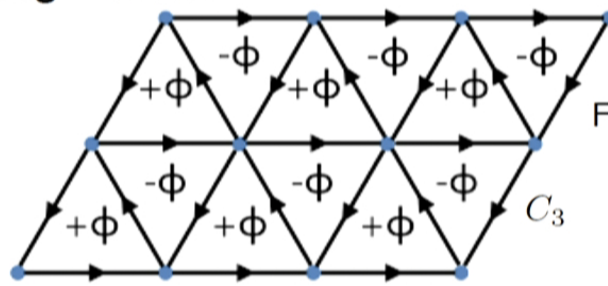
Nearest neighbor Hund's: Ferromagnetic spin-spin coupling

both at order 1% U

U is around 25 meV if dielectric constant is 8.

Trivial Side

Hopping Pattern

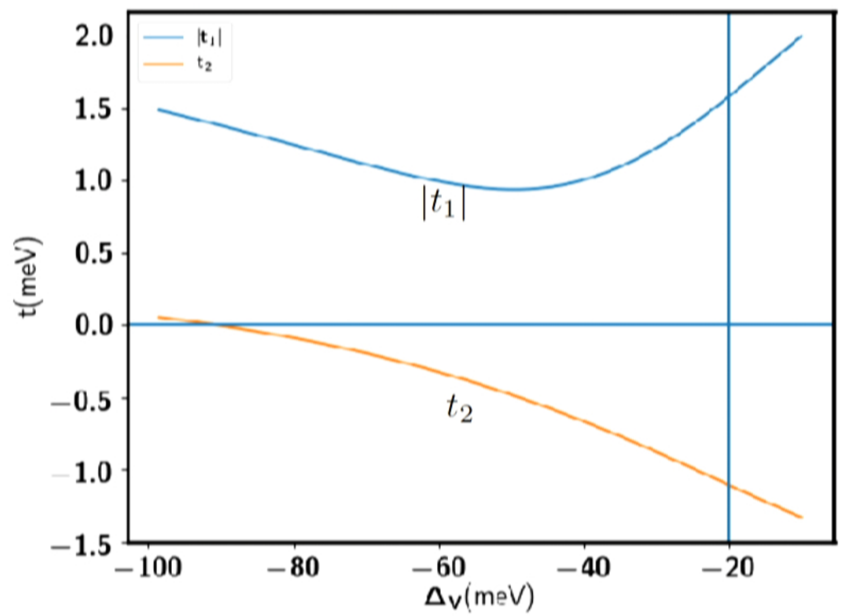


For one valley

Valley-Contrasting Flux

$$\Phi \sim \frac{\pi}{2} - \pi$$

Time Reversal: $\Phi_+ = -\Phi_-$



Vertical line: estimation for potential difference to make bandwidth=U=25 meV

Next Part

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(2) Fractional Filling at Flat Band limit

Trivial Side

Strong Mott Region: U>>t

Number of particles at each site $\nu_T = 1, 2$

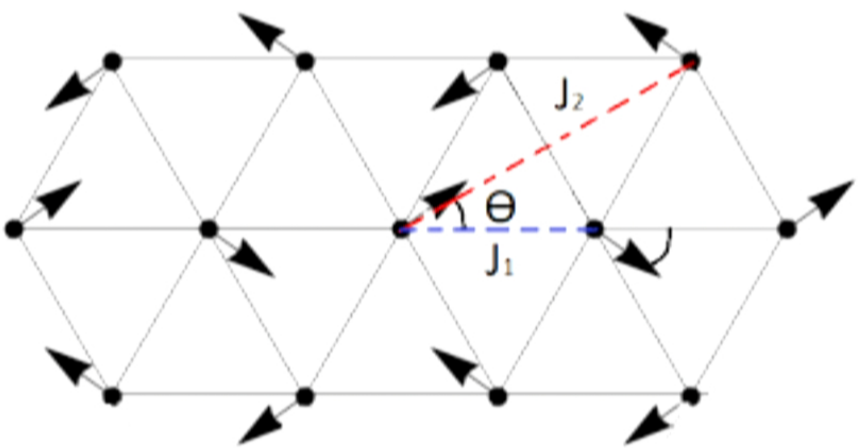
Feng Wang et.al. arxiv:1803.0198

Charge is frozen at each site.

Low energy only has spin-valley neutral degree of freedom

t/U expansion: $J_1 - J_2$ spin-valley model

SU(4) is strongly broken to $U(2)_+ \times U(2)_-$



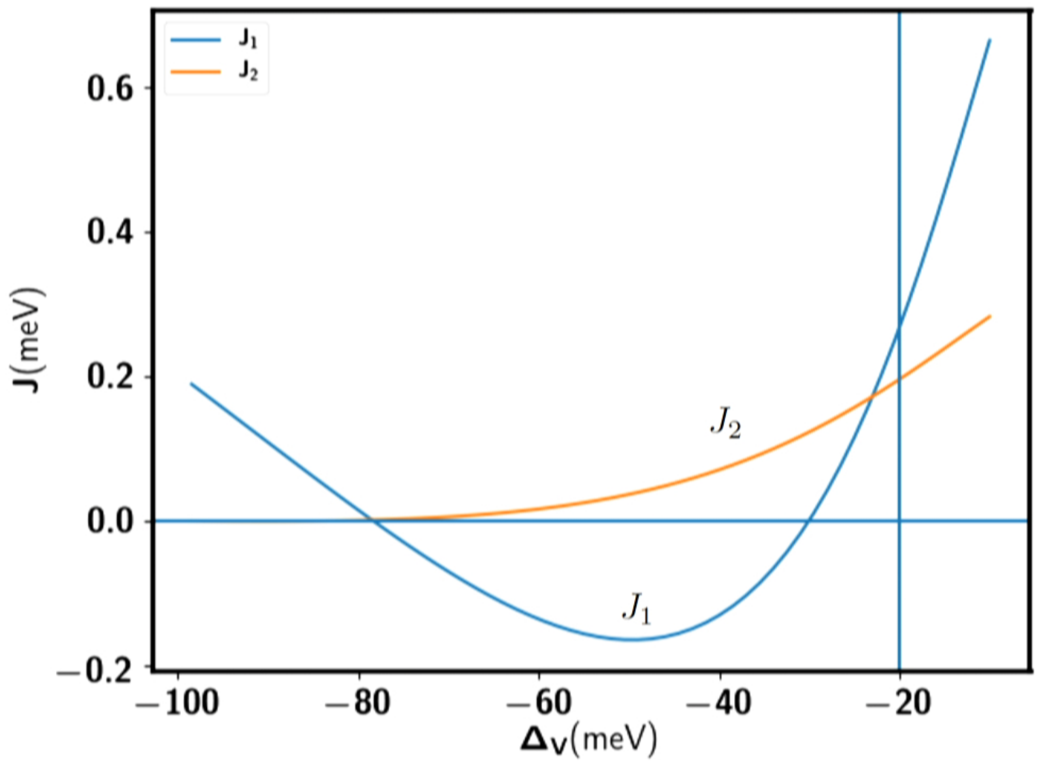
Trivial Side

Ferromagnetic vs Anti-Ferromagnetic

Two Contributions for : J_1

1. Inter-site Hund's: 1% of U

2. Super-exchange: $\frac{t^2}{U} \sim 0.01U$



Strong Mott Insulator: Some Special Cases

DMRG is needed to map out the phase diagram.

Ferromagnetic Region: $J_1 < 0, J_2 \sim 0$

ν_T =2: Spin polarized; Valley singlet

ν_T =1: Spin and valley polarized

Anti-Ferromagnetic Region:

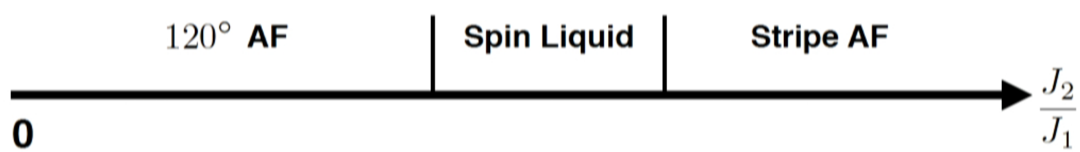
Valley Zeeman coupling: $-g\mu_B B\tau_z$ $g \approx 45$

B=0.2 T: valley splitting 0.4 meV; at order of J

After Valley polarization: spin 1/2 model

Possible U(1) Dirac Spin Liquid!

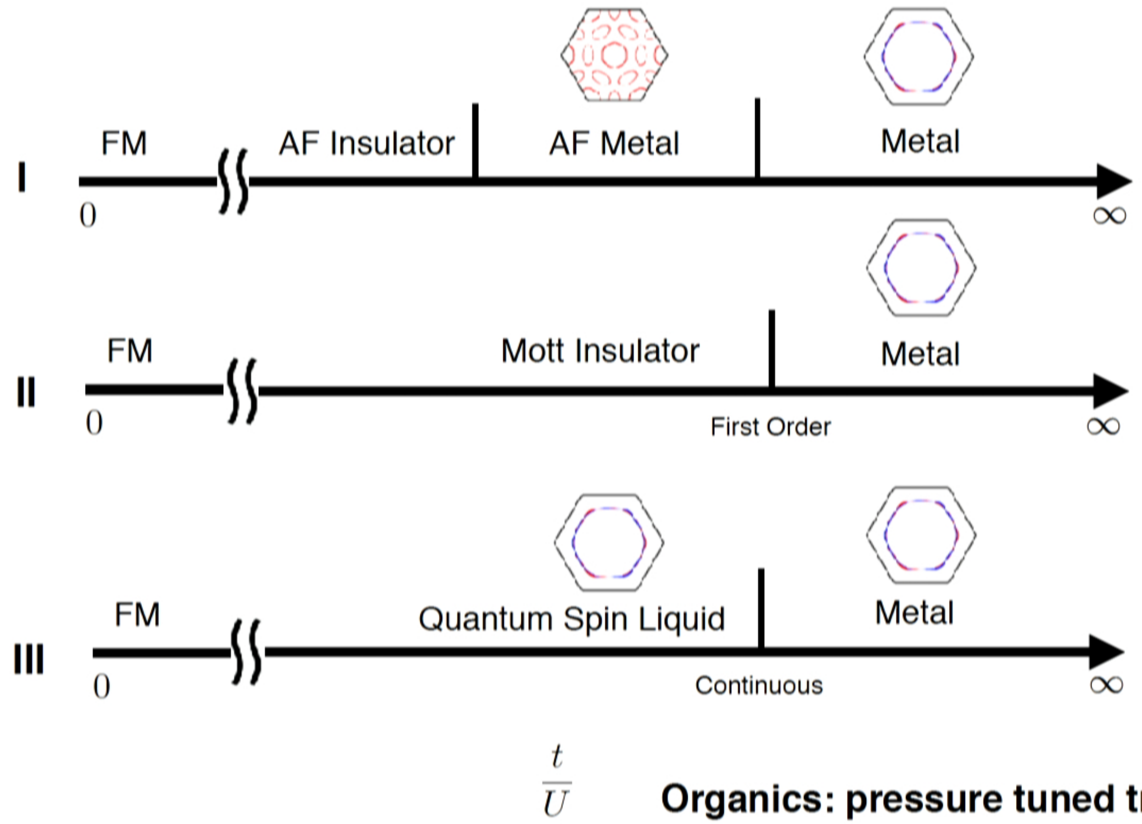
Z. Zhu and S. R. White, Phys. Rev. B 92, 041105 (2015).
W.-J. Hu, et.al., Phys. Rev. B 92, 140403 (2015)
Yasir Iqbal , et.al., Phys. Rev. B 93, 144411 (2016)



Trivial Side

Weak Mott Insulator: Metal-Insulator Transition

Possible Scenarios:



Organics: pressure tuned transition

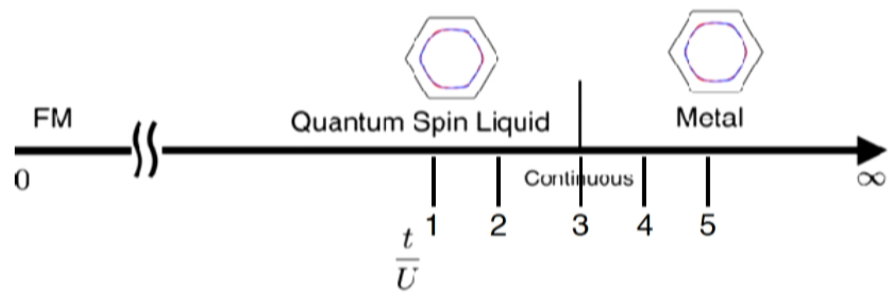
T. Furukawa, et. al. Nature Physics 11, 221 EP (2015)

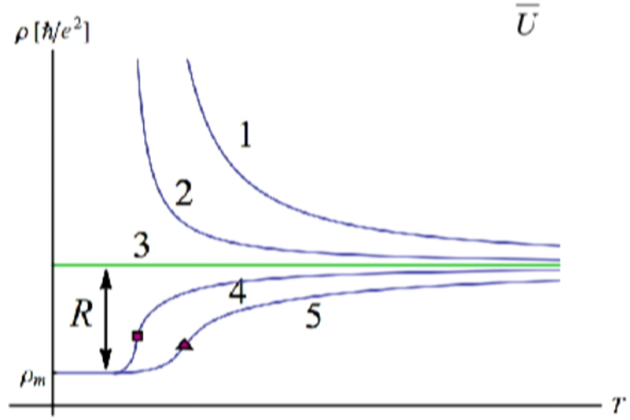
Trivial Side

Continuous Mott Transition

T. Senthil Phys. Rev. B **78**, 045109 (2008)

Experimental Detection: Universal Residual Resistivity Jump





(c)

Witczak-Krempa et.al. , Phys. Rev. B 86, 245102 (2012)

Scaling relation:

$$\rho(T,\delta) - \rho_m = \frac{\hbar}{e^2} G\left(\frac{\delta^{z\nu}}{T}\right)$$

$$z = 1 \ \nu \approx 0.672$$

Chern Side

General Remarks

Y-H. Zhang, D. Mao, C. Yuan, P. Jarillo-Herrero, T. Senthil arxiv:1805.08232

Other Materials: $C = \pm 1, \pm 2, \pm 3$

Twisted Bilayer/Bilayer, Trilayer/Bilayer, Trilayer/Trilayer

Two control variables: potential difference, twist angle: magic angle

Time Reversal Invariant: Two valleys have opposite Chern numbers.

Free fermion level: quantum Valley Hall effect

Strongly Correlated Effects:

Integer ν_T : correlated insulators

Fractional filling?

Chern Side

Quantum Hall Ferromagnetism: Chern Insulator

Focus on $\nu_T = 1$ flat band limit:

Flat band limit: similar to quantum Hall bilayers from opposite magnetic fields.

Two candidates:

Quantum Anomalous Hall Insulator $\sigma_{xy} = 3\frac{e^2}{h}$

Inter-valley-coherent order $\langle c_+^\dagger c_- \rangle \neq 0$

Energy difference:

Hartree Fock

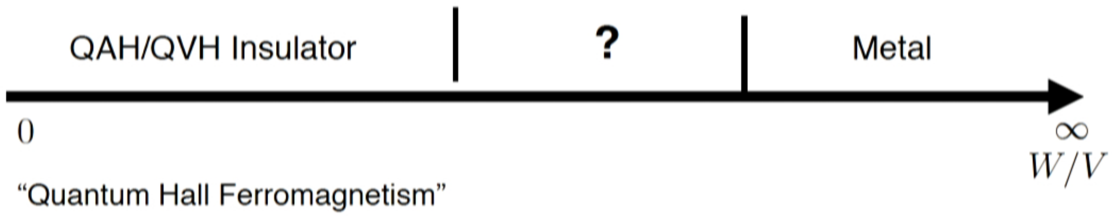
$$\Delta E_{IVC} = H_{F;IVC} - H_{F;0} + H_{K;IVC} - H_{K;0}$$
$$= \frac{1}{4}\sum_{\mathbf{k},\mathbf{q}} V(\mathbf{q})\left(|\lambda_+(\mathbf{k},\mathbf{q})| - |\lambda_-(\mathbf{k},\mathbf{q})|\right)^2$$
$$> 0 \qquad (26)$$

Chern insulator is favored at flat band limit!

Verified by ED calculation, Cécile Repellin, Y-H Zhang, T. Senthil, to appear

Chern Side

Beyond Mott Insulator



What happens at inter-mediate regime?

No simple Lattice model: Wannier Obstruction.

Charge can not be frozen; Non-trivial entanglement between charge-spin

Is a "Quantum Hall Spin Liquid" possible?

A completely new theoretical framework is needed!

A new representation, for example Landau Level?

Two Landau Levels with opposite chiralities.

Summary

We provide models for Trilayer Graphene moire superlattice:

Two sides:

spin-valley Hubbard Model

Nearly flat Chern bands

Correlated Insulators

Trivial Side:

J1-J2 spin-valley model

continuous metal-insulator transition

Chern Side:

Flat band limit: Chern insulator

Inter-mediate Region: need new theoretical framework

Ongoing and Future Work

I. Numerics at integer fillings for both sides.

II. Doped Mott insulator: t-J model

Superconductor

Pseudogap and Strange metal?

III. Fractional filling of Chern side:

Fractional Chern insulator (FCI) or Fractional topological insulator?

Transition between FCI and Fermi Liquid ?

IV. Quantum Hall Bilayers with Opposite Magnetic fields

Composite Fermion Insulator in Opposite-Fields Quantum Hall Bilayers,

Ya-Hui Zhang, arxiv:1810. 03600