GRAPHENE LECTURES

4

Continuum Model

$$\mathcal{H}_{1p} = -i v_F \vec{\tau}\cdot\vec{\nabla} + \frac{v_F k_\theta}{2}\tau^y\gamma^z - \sum_j \left(e^{-i\vec{q}_j\cdot\vec{r}}\, T_j \gamma^+ + h.c.\right)$$

$$\boxed{T_j = v + w\left(\zeta^j \tau^+ + \bar{\zeta}^j \tau^-\right)}$$

<u>BM model</u> $u \sim t'_{AA}/3$ $w \sim t'_{AB}/3$

One can just solve this thing.

$$\mathcal{H}_{1p}|\Psi\rangle = \epsilon|\Psi\rangle$$

Usually do this by expanding in plane waves

$$|\Psi\rangle = \sum_{q\in RLV} |\psi\rangle_{k+q}\, e^{i(k+q)\cdot\vec{x}}$$

← 4-component spinors.

Truncate to $|q| < \Lambda$ & increase Λ to convergence.

Magic happens in this solution. I do not have a simple explanation. But it is not a hard calculation. Enough to take 4 plane wave components already.

Features of the solution

① There are always DPs at K_m, K_m'

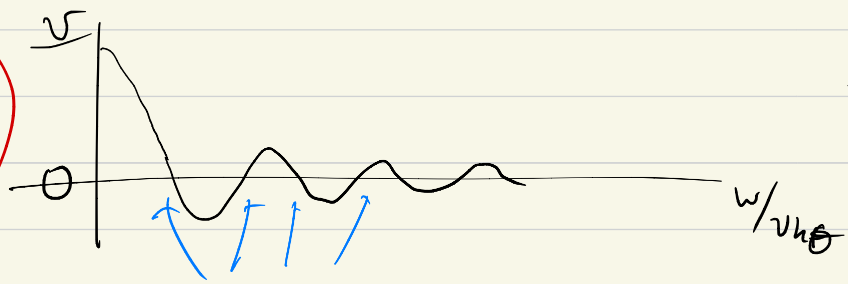
[Check? Data]

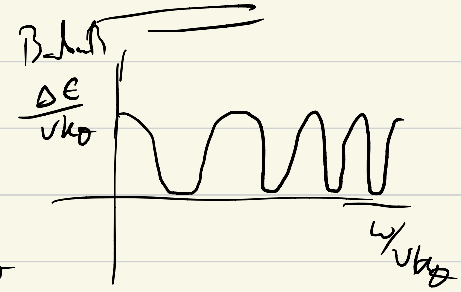
(actually old days → large angles.
→ twisting "decouples" 2 layers.
Corresponds to $\frac{w}{v k_\theta} \ll 1$.)

— Basically BM model preserves $C_2 T R$ → DPs stable.
+ C_3 (can't move)

② Velocity at DPs + Bandwidth shrink + oscillate:

SHOW SLIDES





"magic angles" $\theta \simeq 1.1, 0.5, \ldots$

What is going on? No one really knows!
But we can solve it.

③ Many aspects near magic angles depend on details

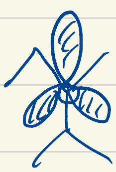
e.g. Separation of flat bands from next bands.
particle/hole symmetry breaking.

SLIDES

④ Subtleties

"Theorist Problem"

- Flat bands mainly have weight in AA region
  "metal puddles"



- But Wannier centers at AB/BA regions.

- Hard to write a single Tight Binding model — "Fragile Topology"

  Po, Vishwanath, Bernevig, ...

Rough issue: bands for 1 valley contain 2 DPs (1 from each layer) both with same winding.

Very hard to find any real physical implication of this.

Definitely no problem w/ continuum model, w/ flat bands, w/ DPs, etc.

Experimentalist Problem

- TBG is not really homogeneous
  - Always variations in twist angle
  - Expt: different contacts can behave differently
  - How does this inhomogeneity (strain) affect the physics?

BUT - Good news

- Still some sharp phenomena
  → Clearly defined insulators, IQHE, SCs ferromagnetism
  → Incoherent "high-T" transport

So: Hopefully as Results, we can still think about uniform systems & capture much of it.

Need to go beyond band theory

- $e^- - e^-$ intn
- e^--phonon intn.

not a priori obvious. BUT probably e-e relevant for insulators.

e-e Interaction [Should also worry about phonons]

Warning: ?100? Theory papers. I've read few.

Graphene: 1-layer.

Low energy Dirac Theory: Basically a FLT

$$H_{eff} = \int d^2x \left\{ -iv\, \psi^\dagger (\tau^z \sigma^x \partial_x + \sigma^y \partial_y)\psi \right.$$
$$\left. + \sum_a g_a\, \psi^\dagger M_a \psi\, \psi^\dagger M_a \psi \right\}$$
$$+ \int d^2x\, d^2x' \frac{e^2}{\varepsilon\sqrt{|x-x'|^2 + a_0^2}}\, e^{-|x-x'|/\xi} (\psi^\dagger\psi)_x (\psi^\dagger\psi)_{x'}$$

$\boxed{\text{Logic}}$ → Integrate out H.E. e^{-1}s ⟹ low-ε eff. field theory.

→ Constraints: Long-Range Coulomb.
If you fix charge density, → extend ε is ε.
then there must still be Coulomb.

[One can do this via scalar potential]

Dimensional analysis: $[g_a] = ?$ $v\,\psi^\dagger \partial_x \psi = E/L^2$ $\Rightarrow \psi^\dagger\psi = \frac{1}{L^2}$

$v/\ell = E$

$[g_a] = E \cdot L^2$ Must be $[g_a] = \frac{e^2 a_0}{\varepsilon}$

Suppose do Grad. exp. $(\psi^\dagger\psi)_{x'} \simeq (\psi^\dagger\psi)_x$

$$\int d^2x' \; \frac{e^2}{\varepsilon\sqrt{|x-x'|^2+a_0^2}} \; e^{-|x-x'|/\xi}$$

$$= \frac{2\pi e^2}{\varepsilon}\int \frac{dx\; x}{\sqrt{x^2+a_0^2}} \; e^{-x/\xi}$$

If $\xi \gg a_0$ dominated by $l x \approx x$.

$$\simeq \frac{2\pi e^2}{\varepsilon}\int dx \; e^{-x/\xi} = \frac{2\pi e^2 \xi}{\varepsilon}$$

We see that the LR part is a factor of $\boxed{\xi/a_0 \text{ larger}}$

This is "dominant term" approx.

Same reason that we can treat e^- gas in semiconductor as though it has just $1/r$ Coulomb.

So to 1st approximation This applies here.

<u>Bilayer</u>

$$H = H_{cm} + \int d^2x\, d^2x' \sum_{\ell\ell'} \frac{e^2 \; e^{-|x-x'|/\xi}}{\varepsilon\sqrt{|x-x'|^2+d^2(1-\delta_{\ell\ell'})}} \psi_\ell^\dagger(x)\psi_\ell(x)\psi_{\ell'}^\dagger(x')\psi_{\ell'}(x')$$

$+$ subdominant SR parts.

ℓ = layers.

d = inter-layer distance. $\simeq 3.4$ Å

c.f. $a = 1.4$ Å

Probably, can neglect "d" in denom. ($d \ll \xi$ still).

$$\text{Then}\quad H' = \int \frac{e^2\, e^{-|x-x'|/\xi}}{\varepsilon |x-x'|} \Big(\underbrace{\sum_\ell \psi_\ell^\dagger \psi_\ell}_{\psi^\dagger\psi}\Big)_x \Big(\underbrace{\sum_{\ell'} \psi_{\ell'}^\dagger \psi_{\ell'}}_{\psi^\dagger\psi}\Big)_{x'}$$

Usually theorists assume this.

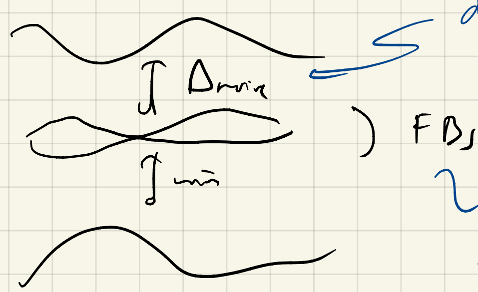
Continuous Symmetries:
- SU(2) Spin rot. ~~\$~~ In each Valley.
- e^- # (Charge) in each valley is conserved

$\iff U(1)_c \times U(1)_v$

BUT 2 valleys are not identical (They are "reflected")

- No continuous rotation of K valley into K' valley.

If "U" $\sim \frac{e^2}{\varepsilon \ell_m} \lesssim \Delta_{moire}$



depends on model!

$\sim$ 10 meV for 1st MA (Theory!)

STM

Project to Flat bands. [From expt → maybe not great?]

$$\psi_{v\sigma}(x) = \sum_{nk} e^{ik\cdot x} \phi_{nkv}(x)\, C_{nv\sigma k}$$

(v: valley, σ: spin)

$$H' = \sum_{\substack{n_1 n_2 n_3 n_4 \\ v v' \sigma \sigma'}} \sum_{k k' q} V_{n_1 \cdots n_4, v v'}(k,k',q)\, C^\dagger_{n_1 v \sigma k} C_{n_2 v \sigma k+q} C^\dagger_{n_3 v' \sigma' k'} C_{n_4 v' \sigma' k'-q}$$

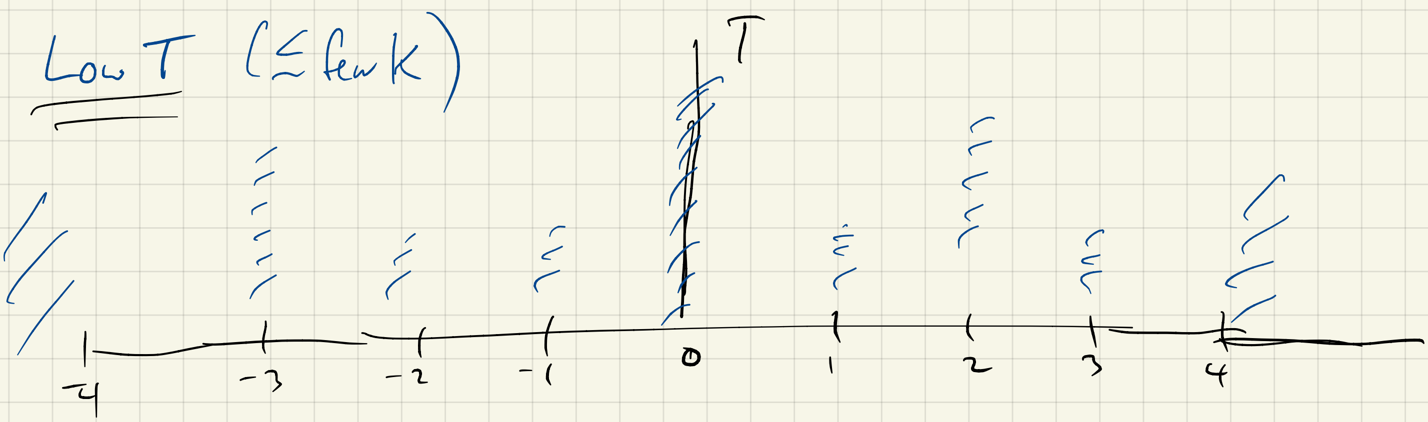
V matrix elements are UGLY & depend on details of bands.

They depend on valley but not spin.

So OK → This is complicated. What do we want to understand?

* Experiments – Jarillo-Herrero, Dean, Young, Efetov, Goldhaber-Gordon, Kim, Tutuc ...

Low T ($\lesssim$ few K)



① Insulators at integer filling of Moiré lattice
– Some seem to be ferromagnetic, in sense of being enhanced by field
others not.

② Superconductivity various places, mostly between the insulators
–

higher T ~ Up to ~200K → Very comprehensive transport study of "incoherent" metal

Tune model system over more than 2 full bandwidth in T
+ over more than bandwidth in $k_B T$

Phonons? e-e?, BoB? Bloch-Gruneisen $T_{BG} = 2\hbar v_p k_F / k_B$ $2k_F$

~10's of K.

Now should discuss "Slater vs. Mott"

- Analogies: Hubbard models
  QH Ferromagnets

How to think about low T?

Two paradigms: Mott-Hubbard System
QH Ferromagnets

- Mott-Hubbard: Large U quenches KE → spin degeneracy
  ≃ local picture
  total band flavor feature

$$H = -\sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j + U \sum_i \sum_{a<b} n_{ia} n_{ib}$$

$U \gg t$ → Heisenberg / t-J → Probably AFs, Maybe QSLs?

all hell breaks loose

- QH FMs ~ "Slater" → S. Girvin, QHE: Novel Excitations & broken Symmetries 1999 on arXiv

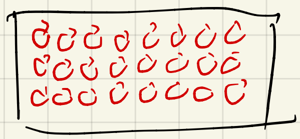
Completely flat band (ie. LL)

$p=1$ ________

$p=0$ ________ $\hbar\omega_c$ ---- $\frac{1}{2}$ filling

1-e States $|p_{LL}; k; \alpha = \uparrow/\downarrow\rangle$

Landau orbit



$$\frac{N}{\text{Area}} = n_e = n_\uparrow + n_\downarrow = \frac{B}{\varphi_0} \times \nu \qquad \nu = 1$$

$$H = \hat{P}_{n=0} H_{Coul} \hat{P}_{n=0}$$

$$H_{Coul} = \frac{1}{2}\int d^2x\, d^2x' \; \hat{n}(x)\, \hat{n}(x')\, V_C(|x-x'|)$$

SU(2) symmetric $[\vec{S}_{TOT}, H] = 0$

Then: Know G.S. $|\Psi_0\rangle$ is eigenstate of $\vec{S}_T^2 = S_T(S_T+1)$ and S_T^z and N

Consider $N = \frac{BL^2}{\varphi_0} = \Phi/\varphi_0$ $\quad \nu_{TOT} = 1$

and Maximal S_T for that N.

ie. $S_T = N/2$

All values of S_T^z have same E

so $S_T^z = N/2$

This state is unique!

$$|\Psi\; S_T = S_T^z = N/2\rangle = \prod_{k \in LLL} c^\dagger_{k\uparrow} |0\rangle$$

So this must be an eigenstate.

Turns out it is also the ground state.

- Basic reason: Short-range part of Coulomb dominates ($V \sim 1/r$) and spin-polarized e^-'s have "correlation hole"
  → Cannot occupy same point (or here, same Landau orbit)

So $\langle \psi | H_c | \psi \rangle$ is minimum.

* This is exact GS. for $P H_c P$. "QH FM"

Context: • Also flat band FMism known in many lattice models — Mielke, Tasaki, Lieb

• Hubbard originally wrote his model as a model for Ferromagnetism (but it is AF at ½ filling)

Lesson for graphene?

* QH Ferromagnets are ideal Hartree Fock ground state. If it is close, HF may be good approx.

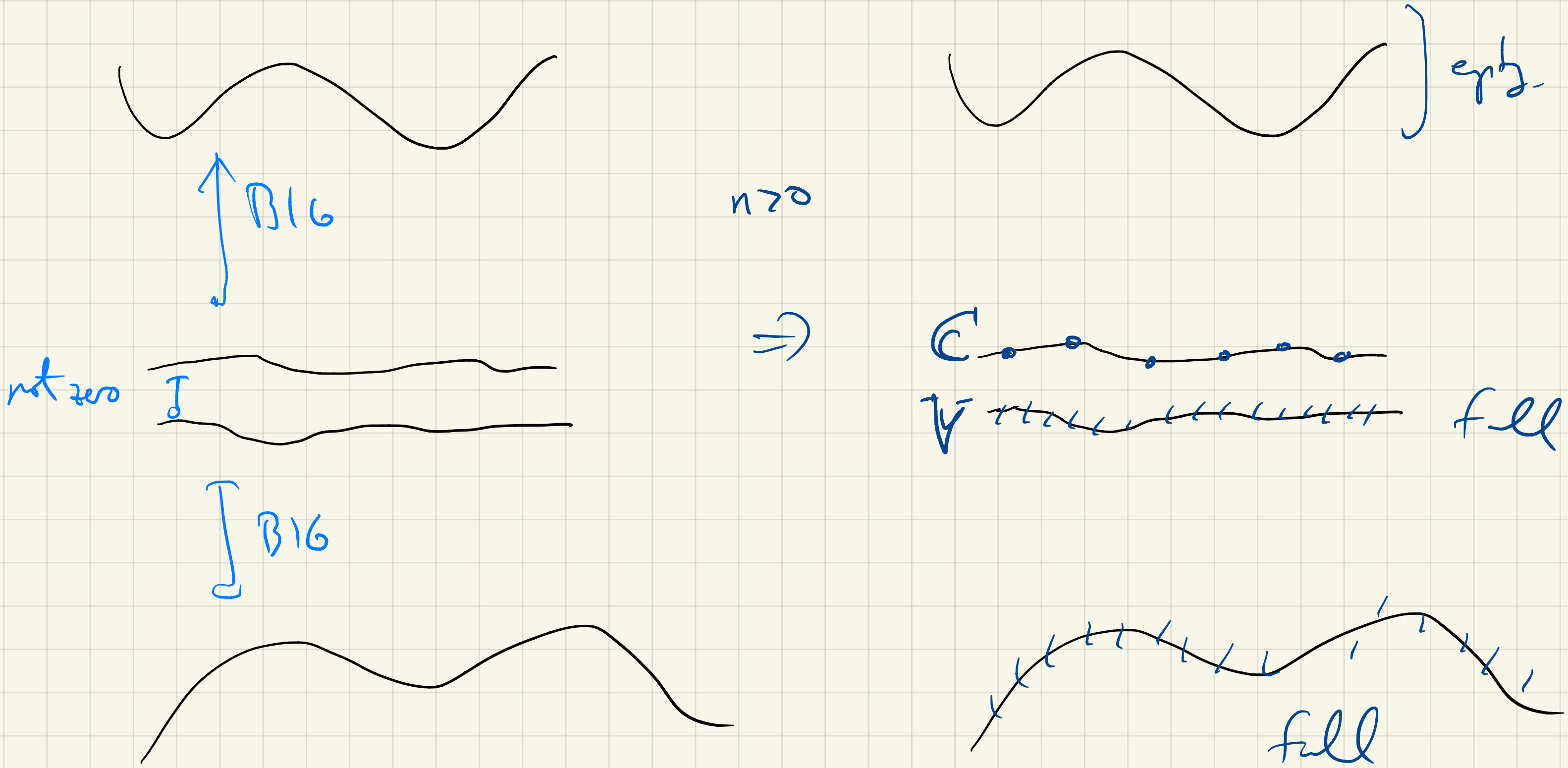
* Simplest HF → Just generalized FMs

spin ⟶ spin × valley

Input: Symmetry TS ($\approx$) $SU(2)_K \times SU(2)_{K'} \times U(1)_K \times U(1)_{K'}$

not $SU(4)$. A bit like bilayer QHFMs

Suppose bands were like this:



→ Project to C band.

Recall S_T, S_T^z, N_K, $N_{K'}$ good QNs
(or S_{Tv}, $S_T^z v$)

$N_K + N_{K'} = N_e$

$n_e = 1$ → 1 e^-/moiré cell → 1 full band

e.g. suppose $n^e_K = 1$, $n^e_{K'} = 0$ $\quad S^z_K = N/2 \quad S_K^{tot} = N/2$

again a unique state.

$$|\psi\rangle = \prod_k C^\dagger_{K,\uparrow}(k)\, |0\rangle$$

Symmetry: K vs K' discrete → DWs
↑ vs → vs ↓ continuous. → Skyrmions/magnons

Such a state is valley-polarized.

Also if C & V are really split, DPs gapped,

so expect valley Chern # ?

∴ May be QAHE

$n_e = 3$ Similar except one band of holes

$$|\psi\rangle = \prod_k C_{K\uparrow}(k) \, |\text{Full}\rangle$$

$n_e = 2$? Could be spin FM.

$$|\psi\rangle = \prod_k C^{(k)}_{K\uparrow} C^{(k)}_{K'\uparrow} \, |0\rangle$$

no valley polarization.

Or valley FM

$$|\psi\rangle = \prod_k C^{\dagger(k)}_{K\uparrow} C^{\dagger}_{K\downarrow}(k) \, |0\rangle$$

no spin polarization

spin singlet.

$n_e = 0$? Just need to separate C & V. Break C_2T or SU(2)

This stuff is rather trivial stealing of old QH ideas.

Even valley dof already done in QHFMs in graphene.

Everything becomes a matter of numbers when we start giving bands width etc.

What's really new?

- Well, I think QHFMs at zero field is new. → QAHE. Can really see both $\sigma = \pm n \frac{e^2}{h}$
- Also, mechanism for QHE is NOT LLs.
  It is really tied to Valley FMism
- Valley FMism is orbital FMism. (Not spin).
- Opportunity to study orbital domain & DWs
  "topological moiré spintronics"