Trions in Twisted Bilayer Graphene

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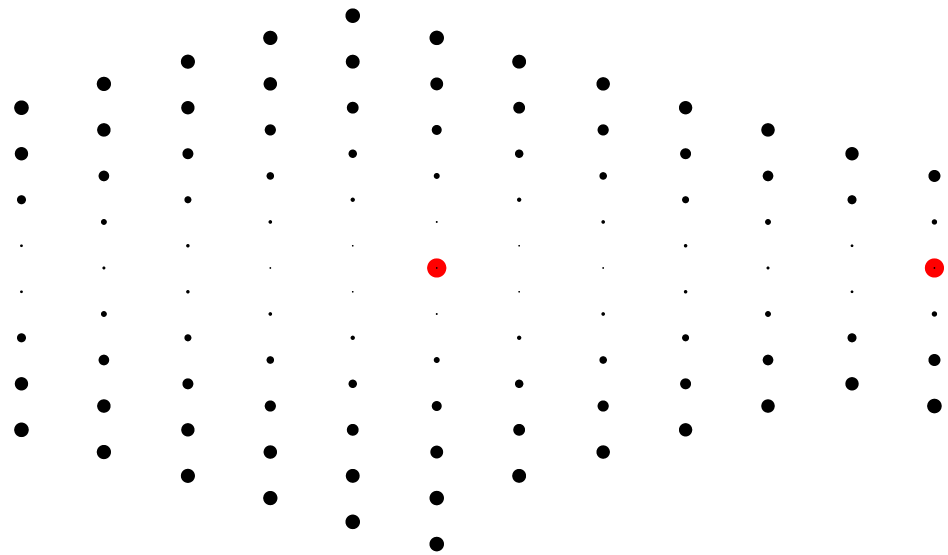

GRS on Correlated Electron Systems,
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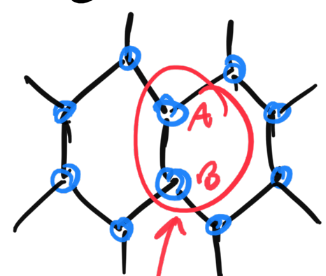
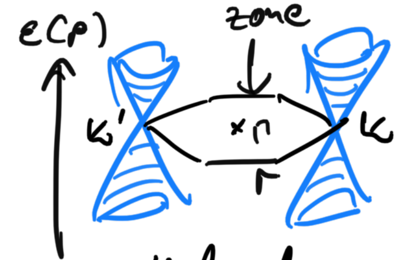
arXiv: 2112.12776
PRB 105, 155135

Twisted Bilayer Graphene

graphene

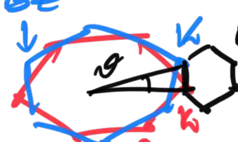


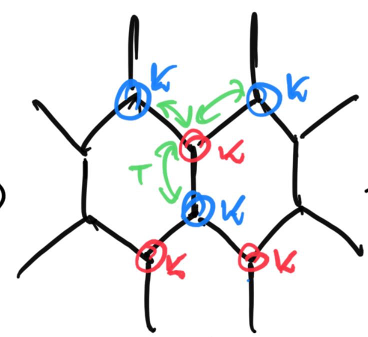
unit cell
(A↑, A↓, B↑, B↓)



4 bands
= 2 × 2
sublattice spin

TBG



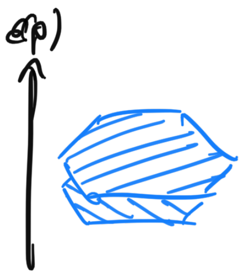


T: inter-layer potential

Bistritzer-MacDonald model

8 flat bands:
= 2 × 2 × 2
layer valley spin

Flat-band projection



$$H = \cancel{H_{kin}} + \sum_{xy} V_{xy}\, \rho_x \rho_y$$

$(c^\dagger_x c_x - \frac{1}{2})$, density

$$\langle \;|H|\; \rangle = 0 + \sum_q V_q\, O_q^\dagger O_q$$

$|u(p)\rangle$: 1-particle Bloch states of flatbands

$$O_q = \sum_{k,\dots} \langle u_{k+q} | u_k \rangle\, \rho_{kq}$$

$k, \dots$: spin, valley, band index

ρ_{kq}: Fourier-transformed density op.

$$= (c^\dagger_{k+q} c_k - \tfrac{1}{2}\delta_{q0})$$

$V_q \geq 0 \rightarrow H$ positive-semidefinite

$$|\Omega_{\alpha\beta}\rangle = \prod_{km} c^\dagger_{km\alpha}\, c^\dagger_{km\beta}\, |0\rangle$$

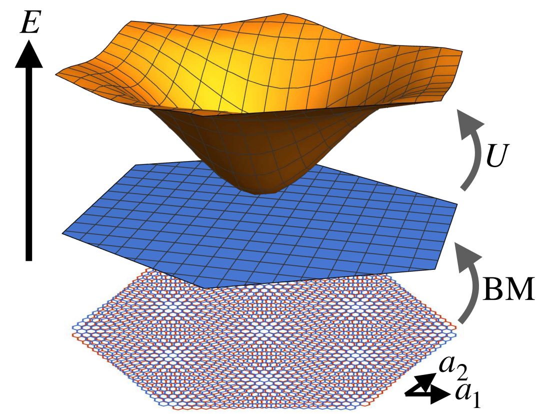
filled 4 of 8 flatbands = charge-neutral

k; m: band index $= 1,2$

α, β: valley-spin index $= (K\uparrow, K\downarrow, K'\uparrow, K'\downarrow)$

ground state $|\Omega\rangle$: $O_q |\Omega\rangle \overset{!}{=} 0$

Quasiparticles

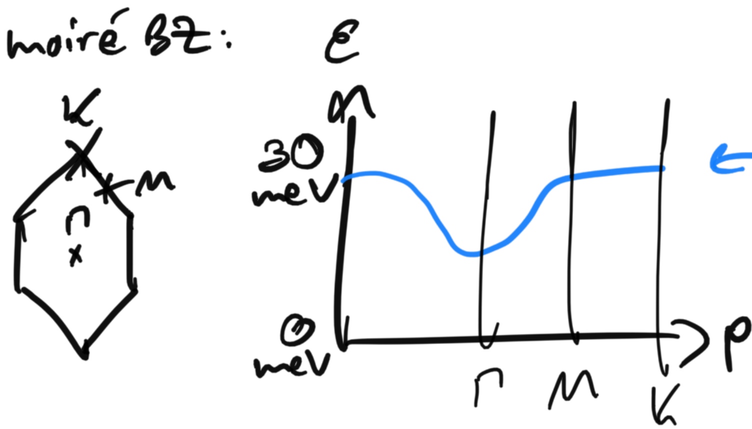


$$H|\Omega\rangle = 0 \;\to\; H c_p^\dagger|\Omega\rangle = [H, c_p^\dagger]|\Omega\rangle$$
$$= \varepsilon_p c_p^\dagger |\Omega\rangle$$

(H preserves total momentum!)

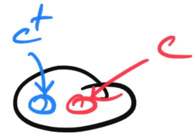
$$e_p = \sum_q V(q)\, |\langle u(p+q)|u(p)\rangle|^2 \qquad |u(p)\rangle : \text{1-particle Bloch states of flatbands}$$

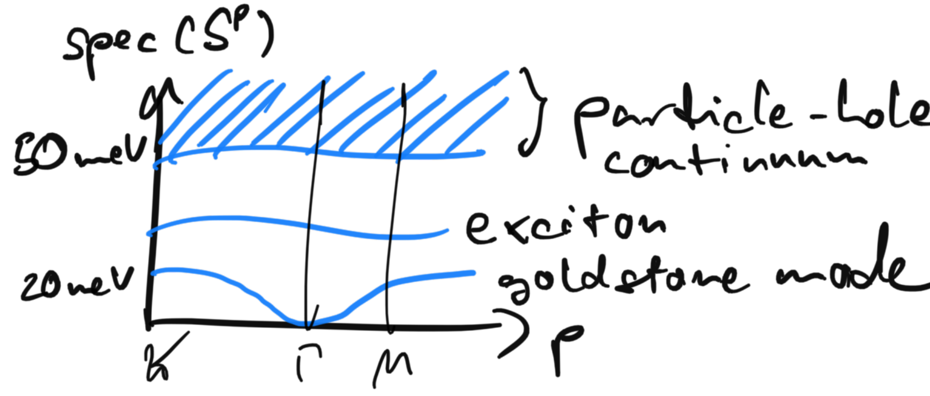
moiré BZ:



Coulomb-induced dispersion (recall $H_{kin} \equiv 0$)

Goldstone modes & Excitons





$$\underbrace{H\, c^\dagger_{k+p}\, c_k}_{\text{total mom.}=p} |\Omega\rangle = [H, c^\dagger_{k+p} c_k] |\Omega\rangle$$

$$= \sum_{k'} S^p_{kk'}\, c^\dagger_{k'+p}\, c_{k'} |\Omega\rangle$$

$$S^p_{kk'} = \delta_{kk'} (\epsilon_{k+p} + \epsilon_k) - 2V(k-k') \langle n(k'+p) | n(k+p) \rangle \cdot \langle n(k) | n(k') \rangle$$

diagonalize $S^p_{kk'}$ = a $N \times N$ matrix

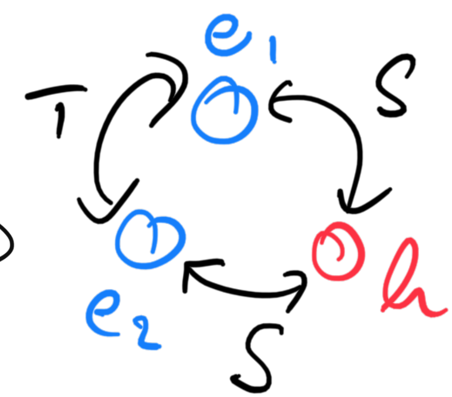
$\uparrow$ # of momenta k = # of unit cells

$\hookrightarrow$ same complexity as single-particle OBC!

Trions

$$H c^{\dagger}_{k_3} c^{\dagger}_{k_2} c_{k_3+k_2-p} |\Omega\rangle$$

$$= \sum_{k_3' k_2'} \underbrace{W^{p}_{k_3 k_2, k_3' k_2'}}_{\text{an } N^2 \times N^2 \text{ matrix}} c^{\dagger}_{k_3'} c^{\dagger}_{k_2'} c_{k_3'+k_2'-p} |\Omega\rangle$$



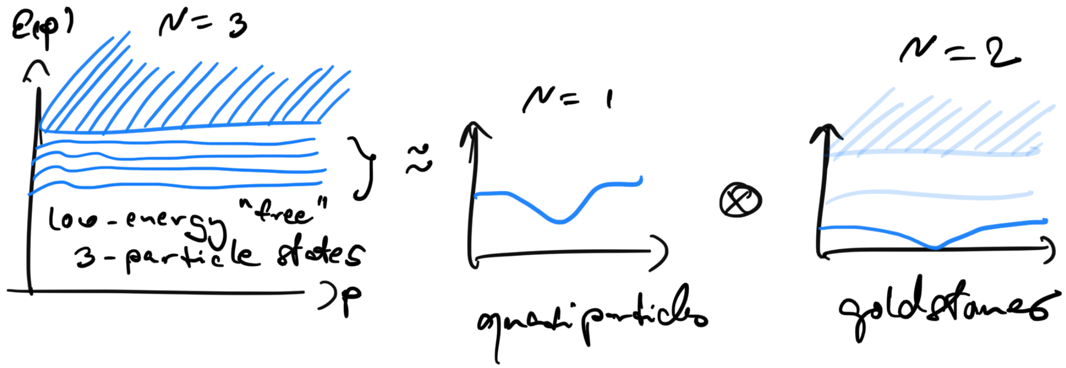
$$W^{p}_{k_3 k_2, k_3' k_2'} = \text{an unholy mess} ☺$$

$T \geq 0$, $S \geq 0$

↳ no Cooper pairs!

$$
\begin{aligned}
&H c^{\dagger}_{\boldsymbol{k}_3,m_3,\eta_3,s_3} c^{\dagger}_{\boldsymbol{k}_2,m_2,\eta_2,s_2} c_{\boldsymbol{k}_2+\boldsymbol{k}_3-\boldsymbol{p},m_1,\eta_1,s_1} |\Psi_0\rangle = \\
&\sum_{\tilde{\boldsymbol{k}}_3,\tilde{\boldsymbol{k}}_2,\tilde{m}_3,\tilde{m}_2,\tilde{m}_1} \Big\{ \delta_{\boldsymbol{k}_3,\tilde{\boldsymbol{k}}_3} \delta_{\boldsymbol{k}_2,\tilde{\boldsymbol{k}}_2} \Big[\underbrace{R^{(\eta_3)}_{\tilde{m}_3,m_3}(\boldsymbol{k}_3) \delta_{\tilde{m}_2,m_2} \delta_{\tilde{m}_1,m_1}}_{\text{Energy 1st electron}} + \underbrace{R^{(\eta_2)}_{\tilde{m}_2,m_2}(\boldsymbol{k}_2) \delta_{\tilde{m}_3,m_3} \delta_{\tilde{m}_1,m_1}}_{\text{Energy 2nd electron}} \\
&+ \underbrace{R^{(\eta_1)}_{m_1,\tilde{m}_1}(\boldsymbol{k}_2+\boldsymbol{k}_3-\boldsymbol{p}) \delta_{\tilde{m}_2,m_2} \delta_{\tilde{m}_3,m_3}}_{\text{Energy hole}} \Big] + \underbrace{2\delta_{\tilde{m}_1,m_1} \delta_{\tilde{\boldsymbol{k}}_2+\tilde{\boldsymbol{k}}_3,\boldsymbol{k}_2+\boldsymbol{k}_3} T^{(\eta_3,\eta_2)}_{-\tilde{\boldsymbol{k}}_2,\tilde{m}_3,\tilde{m}_2;-\boldsymbol{k}_2,m_3,m_2}(\boldsymbol{k}_3+\boldsymbol{k}_2)}_{e_1 - e_2 \text{ repulsion}} \\
&- \underbrace{2\delta_{\tilde{m}_2,m_2} \delta_{\tilde{\boldsymbol{k}}_2,\boldsymbol{k}_2} S^{(\eta_3,\eta_1)}_{\tilde{\boldsymbol{k}}_3+\boldsymbol{k}_2-\boldsymbol{p},\tilde{m}_3,\tilde{m}_1;\boldsymbol{k}_3+\boldsymbol{k}_2-\boldsymbol{p},m_3,m_1}}_{e_1 - h \text{ attraction}} (\boldsymbol{p}-\boldsymbol{k}_2) - \underbrace{2\delta_{\tilde{m}_3,m_3} \delta_{\tilde{\boldsymbol{k}}_3,\boldsymbol{k}_3} S^{(\eta_2,\eta_1)}_{\tilde{\boldsymbol{k}}_2+\boldsymbol{k}_3-\boldsymbol{p},\tilde{m}_2,\tilde{m}_1;\boldsymbol{k}_3+\boldsymbol{k}_2-\boldsymbol{p},m_2,m_1}}_{e_2 - h \text{ attraction}} (\boldsymbol{p}-\boldsymbol{k}_3) \Big\} \\
&c^{\dagger}_{\tilde{\boldsymbol{k}}_3,\tilde{m}_3,\eta_3,s_3} c^{\dagger}_{\tilde{\boldsymbol{k}}_2,\tilde{m}_2,\eta_2,s_2} c_{\tilde{\boldsymbol{k}}_2+\tilde{\boldsymbol{k}}_3-\boldsymbol{p},m_1,\eta_1,s_1} |\Psi_0\rangle
\end{aligned}
$$

Quasiparticle-goldstone approximation



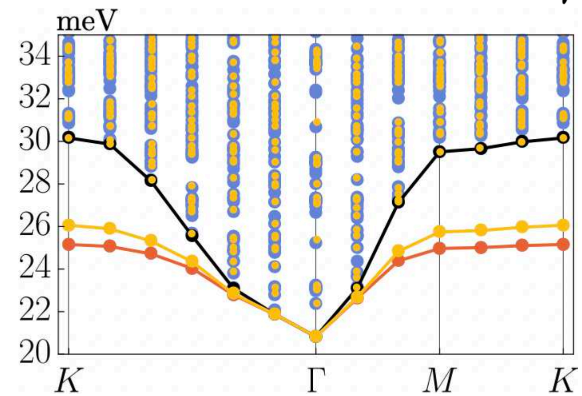
goldstone quasiparticle wave fn's

variational basis $\quad |\,q\,;\,p-q\,\rangle = \sum_k \phi_k^{p-q}\, Q^q\, c^\dagger_q\, c^\dagger_{k+p-q}\, c_k\, |\Omega\rangle$

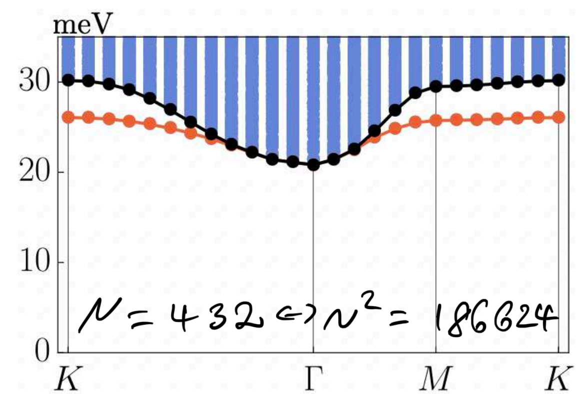
$$\langle q\,;\,p-q\,|\,\hat{H}\,|\,q'\,;\,p-q'\,\rangle \equiv \tilde{\omega}^p_{qq'},$$

an $N \times N$ matrix!

$(N = 108 \Longleftrightarrow N^2 = 11664)$

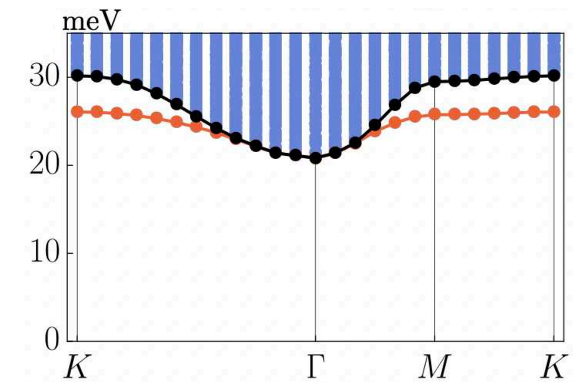


- exact continuum states
- exact trion bound state
- variational solution



Trion bound states

charge neutrality

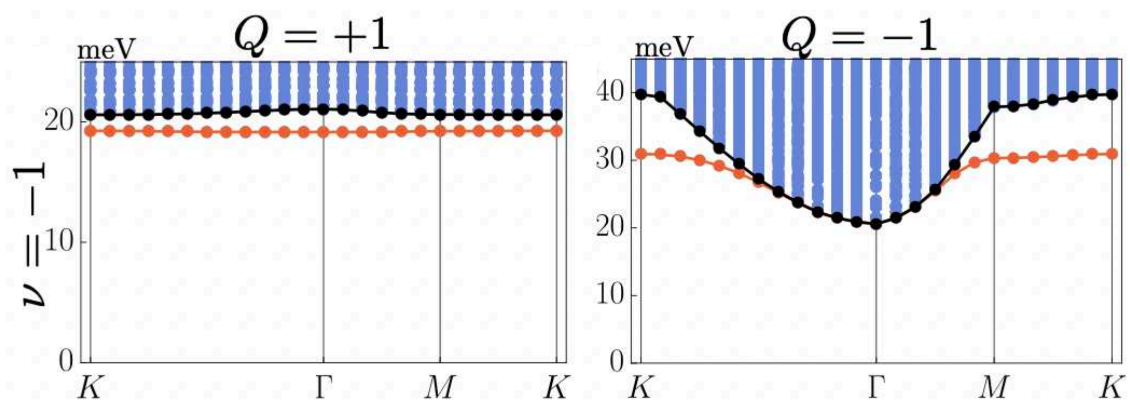


continuum

continuum minimum

Trion bound state

filling $\nu = -1$



See also arXiv: 2112.06835 (E. Khalaf, A. Vishwanath)

Theory for bound states

$|\ \ \rangle$ is an exact eigenstate (goldstone @ Γ = symmetry!)

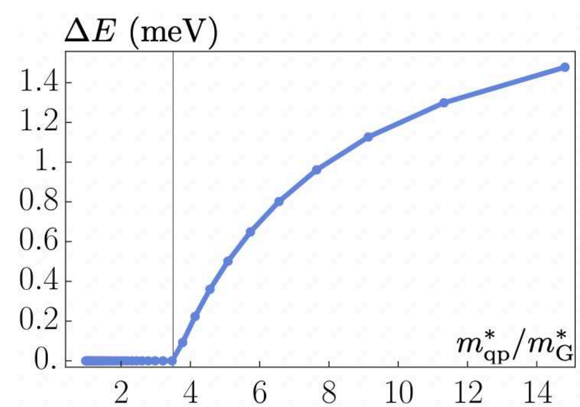
For $m^*_{qp} \ll m^*_G \leftrightarrow |\ \ \rangle_p$ is a good variational basis.

$\langle\ \ |_p \hat{H} |\ \ \rangle_p \sim \frac{1}{N}$

$\hookrightarrow$ no bound state.

quasiparticle (m^*_{qp}) to goldstone (m^*_G) effective mass ratio

(ν, Q)	(0,1)	(0,-1)	(-1,1)	(-1,-1)
$m^*_{\mathrm{qp}}/m_{\mathrm{e}}$	0.098	0.098	13.06	0.048
$m^*_{\mathrm{G}}/m_{\mathrm{e}}$	0.085	0.085	0.088	0.088
$m^*_{\mathrm{qp}}/m^*_{\mathrm{G}}$	1.15	1.15	148	0.54
(ν, Q)	(-2,1)	(-2,-1)	(-3,1)	(-3,-1)
$m^*_{\mathrm{qp}}/m_{\mathrm{e}}$	0.416	0.031	0.211	0.023
$m^*_{\mathrm{G}}/m_{\mathrm{e}}$	0.097	0.097	0.117	0.117
$m^*_{\mathrm{qp}}/m^*_{\mathrm{G}}$	4.28	0.32	1.80	0.20



Thank you for your attention!