Quantum Monte Carlo in momentum space

1. Write down QMC in momentum space
2. Sign problem and sign bounds theory
3. QMC for 2D flat bands systems

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Quantum Monte Carlo in momentum space

1. Write down QMC in momentum space
   - Classical Monte Carlo
   - Some mathematical preparations
   - Review of Hamiltonian in momentum space
   - Determinant QMC in momentum space
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3. QMC for 2D flat bands systems

Classical Monte Carlo

Take classical Ising model as example

$$H = J \sum_{\langle i,j \rangle} s_i s_j \quad (s_i = \pm 1)$$

$$Z = \mathrm{Tr}(e^{-\beta H}) = \sum_{\{s\}} \prod_{\langle i,j \rangle} e^{-\beta J s_i s_j}$$

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}(\hat{O} e^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})} = \sum_{\{s\}} \frac{\prod_{\langle i,j \rangle} e^{-\beta J s_i s_j}}{\sum_{\{s\}} \prod_{\langle i,j \rangle} e^{-\beta J s_i s_j}} O_{\{s\}} = \sum_{\{s\}} W_{\{s\}} O_{\{s\}}$$

Importance sampling

$W_{\{s\}}$ highly non uniform ⇒ Importance sampling

$$P_{s \to s' \neq s} = \frac{1}{N-1} \min\{1, \frac{W_{\{s'\}}}{W_{\{s\}}}\}$$

Detailed balance is promised $P_{s \to s'} W_{\{s\}} = P_{s' \to s} W_{\{s'\}}$, $\sum_{s'} P_{s' \to s} = 1$

Classical Monte Carlo

Once detailed balance is promised $P_{s\to s'}W_{\{s\}} = P_{s'\to s}W_{\{s'\}} \Rightarrow W_{\{s\}} = \sum_{s'} P_{s'\to s}W_{\{s'\}}$, the possibility flowing from s to any s' is equal to the reverse flow, i.e., no possibility redistribution.

$$w_\nu(1) \equiv \begin{pmatrix}0\\0\\1\end{pmatrix}$$

$$w_\mu(2) = \sum_\nu P_{\nu\to\mu} w_\nu(1)$$

$$w_\mu(t_b) = \sum_\nu P_{\nu\to\mu} w_\nu(t_b) = W_\mu$$

We derive the distribution $W_{\{s\}}$ from a random distribution. Measure $O_{\{s\}}$, update, measure $O_{\{s\}}$, update…
Average of all measured $O_{\{s\}}$ will give $\langle \hat{O} \rangle = \sum_{\{s\}} W_{\{s\}} O_{\{s\}}$.

Some mathematical preparations

Trotter decomposition

$$e^{-\beta H} = \prod_t e^{-\Delta t\, H(t)}$$

$$e^{-\Delta t\, H(t)} = e^{-\Delta t\, H_0} e^{-\Delta t\, H_I(t)} + O(\Delta t^2)$$

Hubbard–Stratonovich (HS) transformation

$$e^{a\hat{O}^2} = \int \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2} e^{\sqrt{2a}x\hat{O}} dx \ \ (continuous)$$

$$e^{a\hat{O}^2} = \sum_{l=\pm 1,\pm 2} \frac{1}{4} \gamma(l) e^{\sqrt{a}\eta(l)\hat{O}} + O(a^4) \ \ (discrete)$$

$$\gamma(\pm 1) = 1 + \frac{\sqrt{6}}{3}, \gamma(\pm 2) = 1 - \frac{\sqrt{6}}{3}, \eta(\pm 1) = \pm\sqrt{2\,(3-\sqrt{6})}, \eta(\pm 2) = \pm\sqrt{2\,(3+\sqrt{6})}$$

$(c^\dagger c)^2$ terms

$c^\dagger c$ terms

$$e^{-\beta H} \Rightarrow e^{-H_1} e^{-H_2} \ldots e^{-H_n}$$

Some mathematical preparations

Free fermion partition function

$$Z \equiv \mathrm{Tr}(e^{-M}) = \det(I + e^{-M})$$
$$\mathrm{Tr}(e^{-M_1}e^{-M_2}...e^{-M_n}) = \det(I + e^{-M_1}e^{-M_2}...e^{-M_n})$$

$$e^{-M_1}e^{-M_2}...e^{-M_n} \Rightarrow e^{-M}$$
$$[M_1, M_2] \in M_i,\ M_i = \sum_{k,l} \lambda_{k,l} c_k^\dagger c_l$$

Free fermion Green's function

$$G_{i,j} \equiv \frac{\mathrm{Tr}(c_i c_j^\dagger e^{-M})}{\mathrm{Tr}(e^{-M})} = \delta_{i,j} - \partial_a \ln(\mathrm{Tr}(e^{a c_j^\dagger c_i} e^{-M}))|_{a=0}$$
$$= \delta_{i,j} - \partial_a \mathrm{Tr}_M(\ln(I + e^{a c_j^\dagger c_i} e^{-M}))|_{a=0}$$
$$= \delta_{i,j} - \mathrm{Tr}_M(c_j^\dagger c_i e^{-M}(I + e^{-M})^{-1}) = \delta_{i,j} - \mathrm{Tr}_M(c_j^\dagger c_i(I - (I + e^{-M})^{-1})) = [(I + e^{-M})^{-1}]_{i,j}$$
$$G_{i,j;k,l} \equiv \frac{\mathrm{Tr}(c_i c_j^\dagger c_k c_l^\dagger e^{-M})}{\mathrm{Tr}(e^{-M})} = G_{i,j}G_{k,l} + G_{i,l}(\delta_{k,j} - G_{k,j})\ \ (Wick's\ theorem)$$

Review of Hamiltonian in momentum space

$$H = H_0 + H_I$$

$$H_0 = \sum_{k,m} \varepsilon_{k,m} c^\dagger_{k;m} c_{k;m}$$

$$H_I = \frac{1}{2\Omega} \sum_{q,Q} V(q+Q) \delta\rho_{q+Q} \delta\rho_{-q-Q} = \sum_{|q|\neq 0} \frac{V(q)}{4\Omega} \left[(\delta\rho_q + \delta\rho_{-q})^2 - (\delta\rho_q - \delta\rho_{-q})^2 \right]$$

$$\delta\rho_{q+Q} = \sum_k \sum_{m,n} \lambda_{n,m}(k, k+q+Q) \, (c^\dagger_{k;n} c_{k+q;m} - \mu \delta_{q,0} \delta_{m,n})$$

$$\lambda_{n,m}(k, k+q+Q) \equiv \sum_{K,X} u^*_{K,X;n}(k) u_{K+Q,X;m}(k+q)$$

$$c^\dagger_{k;n} = \sum_{K,X} u_{n;K,X}(k) \, c^\dagger_{k;K,X}$$

Determinant QMC in momentum space

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right) = \mathrm{Tr}\left(\prod_t e^{-\Delta t\, H_0} e^{-\Delta t\, H_I(t)}\right)$$

$$e^{\alpha \hat{O}^2} = \sum_{l=\pm 1,\pm 2} \frac{1}{4}\gamma(l)\, e^{\sqrt{\alpha}\,\eta(l)\hat{O}} + O(\alpha^4)$$

$$= \mathrm{Tr}\left(\prod_t e^{-\Delta t\, H_0} e^{-\Delta t \frac{1}{4\Omega}\sum_{|q|\neq 0} V(q)\left[(\delta\rho_{-q}+\delta\rho_q)^2 - (\delta\rho_{-q}-\delta\rho_q)^2\right]}\right)$$

$$A_q \equiv \sqrt{\frac{\Delta t\, V(q)}{4\Omega}}$$

$$\approx \sum_{\{l_{|q|,t}\}} \prod_t \left[\prod_{|q|\neq 0} \frac{1}{16}\gamma(l_{|q_1|,t})\,\gamma(l_{|q_2|,t})\right] \mathrm{Tr}\left\{\prod_t \left[e^{-\Delta t\, H_0} \prod_{|q|\neq 0} e^{i\eta(l_{|q_1|,t})A_q(\delta\rho_{-q}+\delta\rho_q)} e^{\eta(l_{|q_2|,t})A_q(\delta\rho_{-q}-\delta\rho_q)}\right]\right\}$$

$$\langle \hat{O}\rangle = \frac{\mathrm{Tr}\left(\hat{O}e^{-\beta H}\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)}$$

$$= \sum_{\{l_{|q|,t}\}} \frac{P(\{l_{|q|,t}\})\,\mathrm{Tr}\left[\prod_t \hat{B}_t(\{l_{|q|,t}\})\right] \frac{\mathrm{Tr}\left[\hat{O}\prod_t \hat{B}_t(\{l_{|q|,t}\})\right]}{\mathrm{Tr}\left[\prod_t \hat{B}_t(\{l_{|q|,t}\})\right]}}{\sum_{\{l_{|q|,t}\}} P(\{l_{|q|,t}\})\,\mathrm{Tr}\left[\prod_t \hat{B}_t(\{l_{|q|,t}\})\right]}$$

$$P(\{l_{|q|,t}\}) = \prod_t \left[\prod_{|q|\neq 0} \frac{1}{16}\gamma(l_{|q_1|,t})\,\gamma(l_{|q_2|,t})\right]$$

$$\hat{B}_t(\{l_{|q|,t}\}) = e^{-\Delta t\, H_0} \prod_{|q|\neq 0} e^{i\eta(l_{|q_1|,t})A_q(\delta\rho_{-q}+\delta\rho_q)} e^{\eta(l_{|q_2|,t})A_q(\delta\rho_{-q}-\delta\rho_q)}$$

$\mathrm{Tr}\left[\prod_t \hat{B}_t(\{l_{|q|,t}\})\right]$ is not always

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Avoid sign problem

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}(\hat{O} e^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})}$$

$$= \sum_{\{l_{|q|,t}\}} \frac{P(\{l_{|q|,t}\}) \mathrm{Tr}[\prod_t \hat{B}_t(\{l_{|q|,t}\})] \frac{\mathrm{Tr}[\hat{O} \prod_t \hat{B}_t(\{l_{|q|,t}\})]}{\mathrm{Tr}[\prod_t \hat{B}_t(\{l_{|q|,t}\})]}}{\sum_{\{l_{|q|,t}\}} P(\{l_{|q|,t}\}) \mathrm{Tr}[\prod_t \hat{B}_t(\{l_{|q|,t}\})]}$$

$$\equiv \frac{\sum_l W_l \langle \hat{O} \rangle_l}{\sum_l W_l} = \frac{\frac{\sum_l |\mathrm{Re}(W_l)| \frac{W_l}{|\mathrm{Re}(W_l)|} \langle \hat{O} \rangle_l}{\sum_l |\mathrm{Re}(W_l)|}}{\frac{\sum_l |\mathrm{Re}(W_l)| \frac{W_l}{|\mathrm{Re}(W_l)|}}{\sum_l |\mathrm{Re}(W_l)|}} \equiv \frac{\langle \hat{O} \rangle_{|\mathrm{Re}(W_l)|}}{\langle sign \rangle}$$

$$\mathrm{Tr}(e^{M_1} e^{M_2} \cdots e^{M_n}) = \det(I + e^{M_1} e^{M_2} \cdots e^{M_n})$$

$$D(l) \equiv \mathrm{Tr}[\prod_t \hat{B}_t(\{l_{|q|,t}\})] \equiv \det(D_M)$$

If $\det(D_M) = \det(D_1)\det(D_2) = \det(D_1)\det(D_1^*) > 0$, then no sign problem.

$$\langle sign \rangle = \frac{\sum_l W_l}{\sum_l |\mathrm{Re}(W_l)|} \sim \frac{Z}{Z_{fiction}} \sim e^{-\beta N \Delta f}$$

$$\langle \hat{O} \rangle \sim O(1), \langle sign \rangle \sim e^{-\beta N \Delta f} \Rightarrow \langle \hat{O} \rangle_{|\mathrm{Re}(W_l)|} \sim e^{-\beta N \Delta f}$$

Sign bounds theory

$$D(l) \equiv \mathrm{Tr}\,[\prod_t \hat{B}_t(\{l_{|q|,t}\})] \equiv \det(D_M)$$

$$Z = \sum_l P(l)\,\mathrm{Tr}\,[\prod_t \hat{B}_t(l)] \equiv \langle D \rangle$$

$$\sum_l |\mathrm{Re}(W_l)| = \sum_l P(l)|\mathrm{Re}(D(l))| \leq \sum_l P(l)|D(l)| \leq \sqrt{\sum_l P(l)|D(l)|^2}$$

$$\langle sign \rangle = \frac{\sum_l W_l}{\sum_l |Re(W_l)|} = \frac{Z}{?}$$

$$\langle sign \rangle \geq \frac{\langle D \rangle}{\langle |D| \rangle} \equiv \langle sign \rangle_{|D|}$$

$$\langle sign \rangle \geq \frac{\langle D \rangle}{\sqrt{\langle |D|^2 \rangle}} \equiv \langle sign \rangle_{|D|^2}$$

⇩ ⇩

$\langle |D| \rangle$ $\sqrt{\langle |D|^2 \rangle}$ $\langle (|D| - \langle |D| \rangle)^2 \rangle \geq 0$

If $\langle |D| \rangle$ or $\langle |D|^2 \rangle$ can be written back to non-decoupled Hamiltonian, one can derive the bounds behavior of $\langle sign \rangle$ according to partition functions of target/original system and reference system.

$$\langle sign \rangle \geq \frac{Z_D}{Z_{|D|}} \text{ or } \langle sign \rangle \geq \frac{Z_D}{Z_{|D|^2}}$$

Two corollaries for two reference systems

Corollary I: If D is real for every configuration (e.g., decoupled Hamiltonian is real), $|D|^2 = D^2$

$$D(l)^2 = \det\begin{pmatrix} D_M & 0 \\ 0 & D_M \end{pmatrix} = \mathrm{Tr}\left[\prod_t \hat{B}_{t,+}(l)\hat{B}_{t,-}(l)\right]$$

$$H \to H_{|D|^2} \ by \ c_\alpha^\dagger c_\beta \to \sum_{s=+,-} c_{\alpha,s}^\dagger c_{\beta,s}$$

$$\langle sign\rangle \geq \frac{Z_D}{Z_{|D|^2}}$$

At low temperature limit,

$$\langle sign\rangle \geq \frac{g_D e^{-\beta\,(E_D - E_{|D|^2}/2)}}{\sqrt{g_{|D|^2}}}$$

Corollary II: For a Hamiltonian like

$$H = K + \sum_A (A - \mu_A)^2$$

where A and K are fermion bilinears and μ_A is real constant number. If for a certain group of μ_A, there is no sign problem, one can take $Z_{|D|}$ as a reference system (This can be seen by noticing μ_A only contributes a phase in D).

$$\langle sign\rangle \geq \frac{g_D e^{-\beta(E_D - E_{|D|})}}{g_{|D|}}$$

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Superconductor within moiré flat bands

General interaction in density channel

$$H_I = \frac{1}{2\Omega}\sum_G \sum_{q\in mBZ} V(q+G)\delta\rho_{q+G}\delta\rho_{-q-G}$$

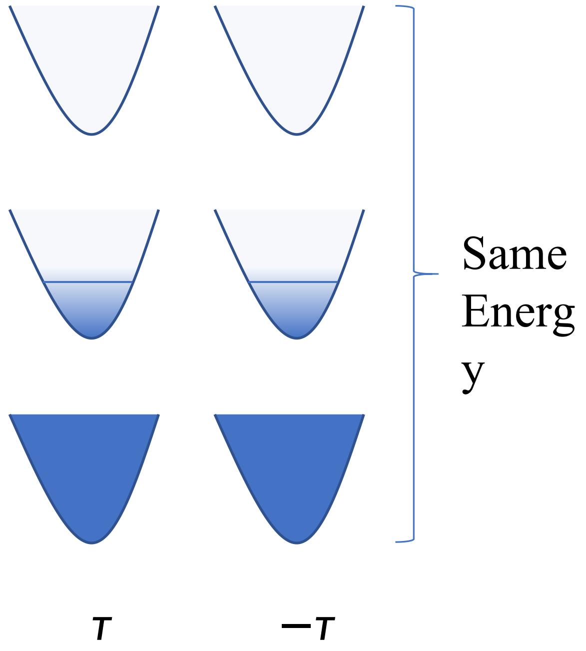
$$\delta\rho_{q+G} = \sum_{k,X}(f^\dagger_{k,\tau,X} f_{k+q+G,\tau,X} + f^\dagger_{k,-\tau,X} f_{k+q+G,-\tau,X})$$

$$\delta\rho_{q+G}\delta\rho_{-q-G} = \mathrm{F}_\tau \mathrm{F}_\tau + \mathrm{F}_{-\tau}\mathrm{F}_{-\tau} + \mathrm{F}_\tau \mathrm{F}_{-\tau} + \mathrm{F}_{-\tau}\mathrm{F}_\tau$$

Introduce inter-valley attractive interaction

$$\delta\rho_{q+G}\delta\rho_{-q-G} = \mathrm{F}_\tau \mathrm{F}_\tau + \mathrm{F}_{-\tau}\mathrm{F}_{-\tau} - \mathrm{F}_\tau \mathrm{F}_{-\tau} - \mathrm{F}_{-\tau}\mathrm{F}_\tau$$

$$\delta\rho_{q+G} = \sum_{k,X}(f^\dagger_{k,\tau,X} f_{k+q+G,\tau,X} - f^\dagger_{k,-\tau,X} f_{k+q+G,-\tau,X})$$



No sign problem $SU(2) \Rightarrow$ Exact solution

Superconductor within moiré flat bands

No sign problem

$$\delta\rho_{q+G} = \sum_{k,m,n} \left(\lambda_{m,n,\tau}(k, k+q+G)\, c^\dagger_{k,m,\tau} c_{k+q,n,\tau} - \lambda_{m,n,-\tau}(k, k+q+G)\, c^\dagger_{k,m,-\tau} c_{k+q,n,-\tau}\right)$$

$$\delta\rho_{q+G,-\tau} \equiv - \sum_{k,m,n} \lambda_{m,n,-\tau}(k, k+q+G)\, c^\dagger_{k,m,-\tau} c_{k+q,n,-\tau}$$

$$= - \sum_{k,m,n} \lambda^*_{m,n,\tau}(k, k-q-G)\, c^\dagger_{-k,m,-\tau} c_{-k+q,n,-\tau}$$

$$= - \sum_{k,m,n} \lambda^*_{m,n,\tau}(k, k-q-G)\, \tilde{c}^\dagger_{k,m,-\tau} \tilde{c}_{k-q,n,-\tau} = - \delta\rho^*_{-q-G,\tau}$$

$$\hat{B}_{t,\tau}(\{l_{|q|,t}\}) = e^{-\Delta t\, H_{0,\tau}} \prod_{|q|\neq 0} e^{i\eta(l_{|q_1|,t}) A_q (\delta\rho_{-q,\tau} + \delta\rho_{q,\tau})} e^{\eta(l_{|q_2|,t}) A_q (\delta\rho_{-q,\tau} - \delta\rho_{q,\tau})}$$

$$\hat{B}_{t,-\tau}(\{l_{|q|,t}\}) = e^{-\Delta t\, H_{0,-\tau}} \prod_{|q|\neq 0} e^{-i\eta(l_{|q_1|,t}) A_q (\delta\rho^*_{-q,\tau} + \delta\rho^*_{q,\tau})} e^{\eta(l_{|q_2|,t}) A_q (\delta\rho^*_{-q,\tau} - \delta\rho^*_{q,\tau})}$$

Time reversal requires

$$\lambda_{m,n,-\tau}(k, k+q+G) = \lambda^*_{m,n,\tau}(-k, -k-q-G)$$

$$\tilde{c}^\dagger_{k,m,-\tau} \equiv c^\dagger_{-k,m,-\tau}$$

$$= \hat{B}^*_{t,\tau}(\{l_{|q|,t}\})$$

$$D(l) \equiv \mathrm{Tr}\left[\prod_t \hat{B}_t(\{l_{|q|,t}\})\right] \equiv \det(D_M)$$

$\det(D_M) = \det(B_\tau)\det(B^*_\tau) > 0$, no sign problem.

Superconductor within moiré flat bands

SU(2) symmetry

Define a pair operator

$$\Delta^{\dagger} = \sum_{k} c_{k,\tau}^{\dagger} c_{-k+Q,-\tau}^{\dagger}$$

$$[\Delta^{\dagger}, \delta\rho_{q+G}] = [\sum_{k'} c_{k',\tau}^{\dagger} c_{-k'+Q,-\tau}^{\dagger}, \sum_{k} (\lambda_{\tau}(k, k+q+G) c_{k,\tau}^{\dagger} c_{k+q,\tau} - \lambda_{-\tau}(k, k+q+G) c_{k,-\tau}^{\dagger} c_{k+q,-\tau})]$$
$$= \sum_{k} (\lambda_{-\tau}(k-Q, k+q+G-Q) - \lambda_{-\tau}(k, k+q+G)) c_{k,-\tau}^{\dagger} c_{-k-q+Q,\tau}^{\dagger}$$

One can see when $Q = 0$, $[\Delta^{\dagger}, \delta\rho_{q+G}] = 0$, which means $[\Delta^{\dagger}, H_I] = [\Delta, H_I] = 0$.

After computing $[\Delta, \Delta^{\dagger}] = N - \hat{N}$, we find SU(2) generators

$$\sigma_x = \Delta + \Delta^{\dagger}$$
$$\sigma_y = i(\Delta - \Delta^{\dagger})$$
$$\sigma_z = \hat{N} - N$$

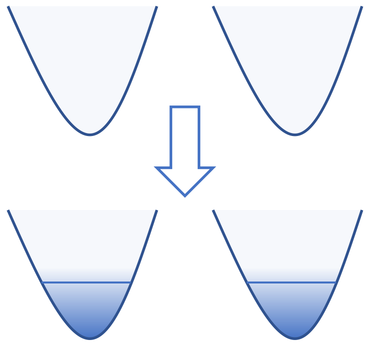
$$[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k$$

Superconductor within moiré flat bands

By noticing $|0\rangle$ and $|2N\rangle$ are two obvious ground states for this positive semi-definite Hamiltonian

$$H_I = \frac{1}{2\Omega}\sum_G \sum_{q\in mBZ} V(q+G)\delta\rho_{q+G}\delta\rho_{-q-G}$$

$$\delta\rho_{q+G} = \sum_{k,m,n} (\lambda_{m,n,\tau}(k,k+q+G)c^\dagger_{k,m,\tau}c_{k+q,n,\tau} - \lambda_{m,n,-\tau}(k,k+q+G)c^\dagger_{k,m,-\tau}c_{k+q,n,-\tau})$$



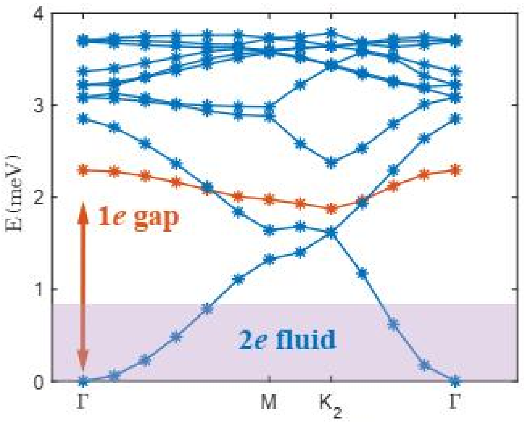
One can see $(\Delta^\dagger)^n|0\rangle$ is also a ground state. The degeneracy of ground state will be $N+1$.

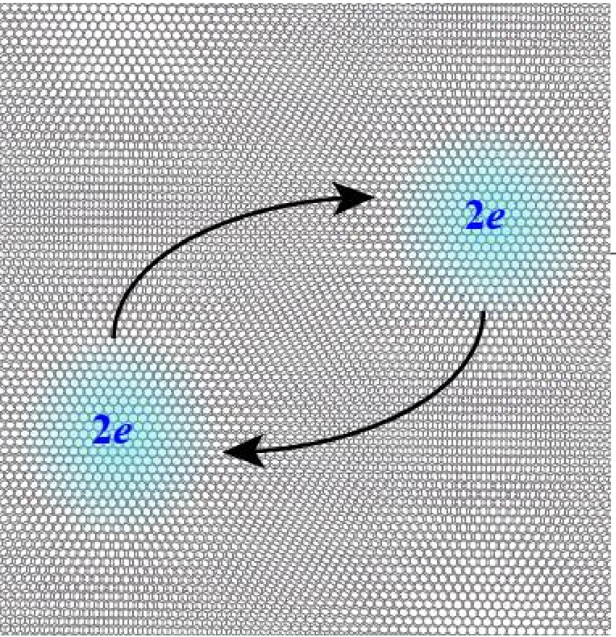
Besides, one can diagonalize this Hamiltonian in single-particle subspace

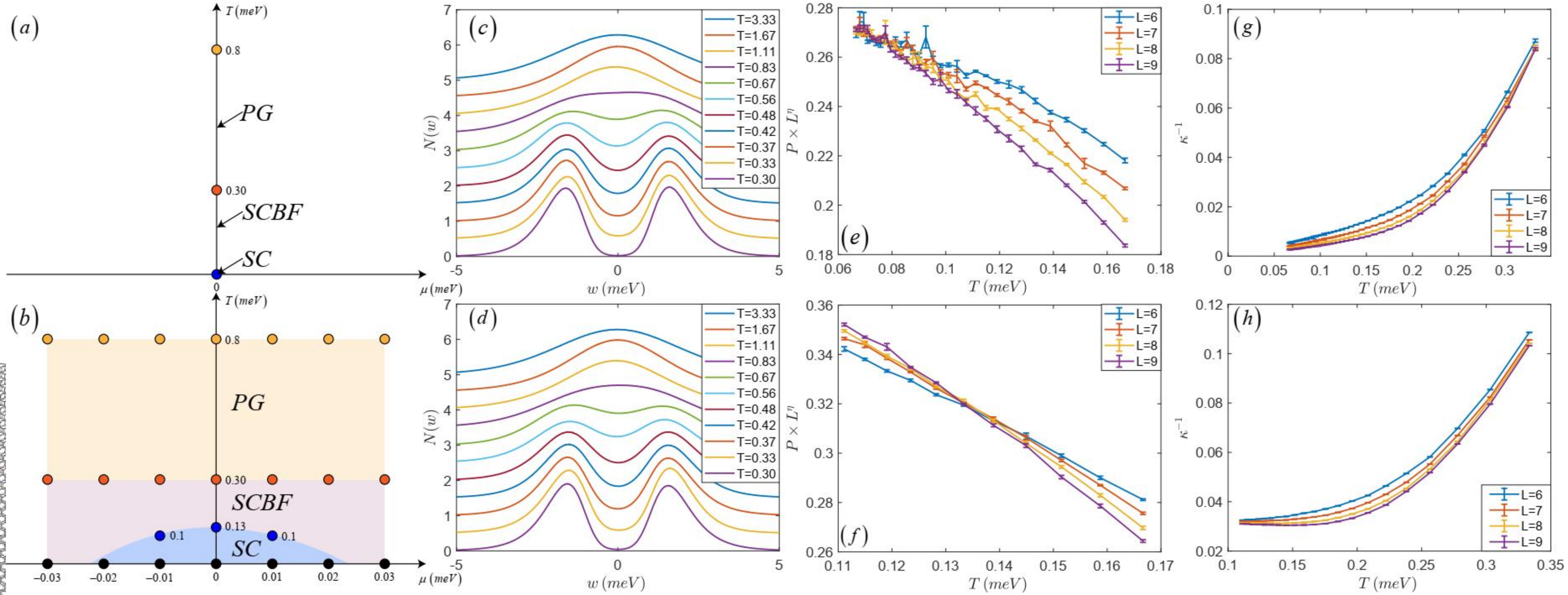
$$H_{I_{sub}} = \frac{1}{2\Omega}\sum_{q,G} V(q+G) \sum_{k,m,n,n',\tau} \lambda_{m,n',\tau}(k,k+q+G)\lambda_{n',n,\tau}(k+q+G,k)c^\dagger_{k,m,\tau}c_{k,n,\tau}$$

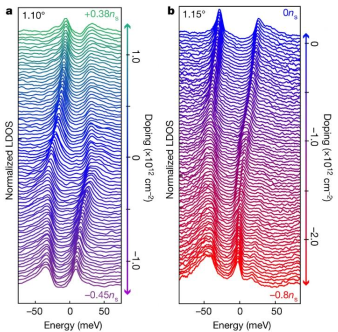
Again, $(\Delta^\dagger)^n|1\rangle$ will give all single-particle excitations

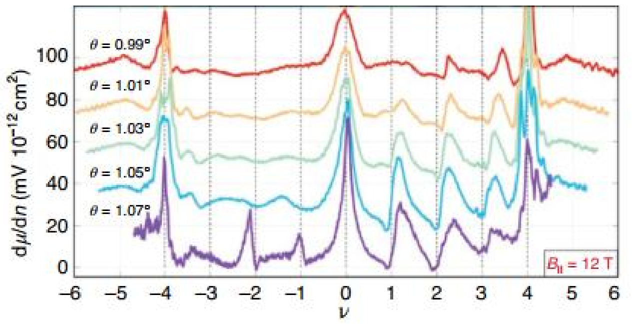
Superconductor within moiré flat bands











TBG in charge neutrality

Sign structure

Degrees of freedom	Kinetic terms	Sign Structure
Single valley single spin	No	Real
Single valley double spin	No	Non-negative
Double valley single spin	Flat bands	Non-negative
Double valley double spin	Flat bands	Non-negative

$$H_I = \frac{1}{2\Omega} \sum_{G} \sum_{q \in mBZ} V(q+G)\,\delta\rho_{q+G}\,\delta\rho_{-q-G}$$

$$\delta\rho_{q+G} = \sum_{s,\tau} \delta\rho_{q+G,s,\tau} = \delta\rho^{\dagger}_{-q-G}$$

$$\delta\rho_{q+G,s,\tau} = \sum_{k} \sum_{n,m} \lambda_{n,m,\tau}(k, k+q+G)\,\left(c^{\dagger}_{k,n,s,\tau} c_{k+q,m,s,\tau} - \frac{1}{2}\delta_{q,0}\delta_{m,n}\right)$$

TBG in charge neutrality

$$\mathrm{Tr}\left(e^{M_1}e^{M_2}\cdots e^{M_n}\right) = \det\left(I + e^{M_1}e^{M_2}\cdots e^{M_n}\right)$$

$$\widehat{B}_t(\{l_{|q|,t}\}) = e^{-\Delta t\, H_0} \prod_{|q|\neq 0} e^{i\eta(l_{|q_1|,t})A_q(\delta\rho_{-q}+\delta\rho_q)} e^{\eta(l_{|q_2|,t})A_q(\delta\rho_{-q}-\delta\rho_q)}$$

When $H_0 = 0$,

$$\mathrm{Tr}\left[\prod_t \widehat{B}_t(\{l_{|q|,t}\})\right] = e^{-\frac{1}{2}\sum_j \mathrm{Tr}(M_j)} \det\left(I + e^{M_1}e^{M_2}\cdots e^{M_n}\right)$$

Define $U = e^{M_1}e^{M_2}\cdots e^{M_n}$, $\det(U) = e^{\sum_j \mathrm{Tr}(M_j)} = e^{\sum_a i\lambda_a} = e^{i\Gamma}$

$$e^{-i\frac{\Gamma}{2}}\det(I+U) = e^{-i\frac{\Gamma}{2}}\prod_a\left(1+e^{i\lambda_a}\right)$$

For any term $e^{i\left(\sum_{k\in A}\lambda_k - \frac{\Gamma}{2}\right)}$, there is always a term $e^{i\left(\sum_{k\notin A}\lambda_k - \frac{\Gamma}{2}\right)} = e^{i\left(-\sum_{k\in A}\lambda_k + \frac{\Gamma}{2}\right)}$. Add all terms together,

$$Tr\left[\prod_t \widehat{B}_t(\{l_{|q|,t}\})\right] = e^{-i\frac{\Gamma}{2}}\det(I+U) = \sum_A 2\cos\left(\sum_{k\in A}\lambda_k - \frac{\Gamma}{2}\right)$$

Real!

TBG in charge neutrality

$$\delta\rho_{q+G,s,\tau} = \sum_k \sum_{n,m} \lambda_{n,m,\tau}(k, k+q+G)\left(c^\dagger_{k,n,s,\tau} c_{k+q,m,s,\tau} - \frac{1}{2}\delta_{q,0}\delta_{m,n}\right)$$

$\lambda_{n,m,\tau}(k-G, k+q) = \lambda_{n,m,\tau}(k, k+q+G)$	Translation
$\lambda^*_{n,m,\tau}(k, k+q+G) = \lambda_{m,n,\tau}(k+q+G, k)$	Hermite
$\lambda_{n,m,\tau}(k, k+q+G) = m * n * \lambda_{-n,-m,-\tau}(k, k+q+G)$	$C_{2z}P$

$$\delta\rho_{q+G,s,-\tau} = \sum_k \sum_{n,m} \lambda_{n,m,-\tau}(k, k+q+G)\left(c^\dagger_{k,n,s,-\tau} c_{k+q,m,s,-\tau} - \frac{1}{2}\delta_{q,0}\delta_{m,n}\right)$$

$$= \sum_k \sum_{n,m} -m * n * \lambda_{n,m,\tau}(k, k+q+G)\left(c_{k+q,-m,s,-\tau} c^\dagger_{k,-n,s,-\tau} - \frac{1}{2}\delta_{q,0}\delta_{m,n}\right)$$

$$= \sum_k \sum_{n,m} -\lambda^*_{m,n,\tau}(k, k-q-G)\left(\tilde{c}^\dagger_{k,m,s,-\tau} \tilde{c}_{k-q,n,s,-\tau} - \frac{1}{2}\delta_{q,0}\delta_{m,n}\right)$$

$$= -\delta\rho^*_{-q-G,s,\tau}$$

$\Longrightarrow$ $\hat{B}_{t,-\tau} = \hat{B}^*_{t,\tau}$ $\Longrightarrow$ $\mathrm{Tr}\left[\prod_t \hat{B}_t(\{l_{|q|,t}\})\right] = D_\tau D_{-\tau} = D_\tau D^*_\tau$

Non-negative!

TBG in other integer fillings

Find a ground state with 0 energy

$$H_I = \frac{1}{2\Omega}\sum_G \sum_{q\in mBZ} V(q+G)\,\delta\rho_{q+G}\,\delta\rho_{-q-G}$$

$$\delta\rho_{q+G} = \sum_{k,m} \lambda_{m,\tau}(k,k+q+G)\left(c^\dagger_{k,m,s,\tau}c_{k+q,m,s,\tau} + c^\dagger_{k,m,-s,\tau}c_{k+q,m,-s,\tau} + \tilde{c}^\dagger_{k,m,s,-\tau}\tilde{c}_{k+q,m,s,-\tau} + \tilde{c}^\dagger_{k,m,-s,-\tau}\tilde{c}_{k+q,m,-s,-\tau} - \frac{v+4}{2}\delta_{q,0}\right)$$

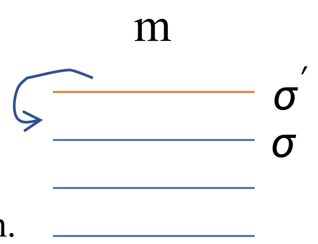
Full fill n Chern bands is one of ground states

$\delta\rho_{q+G}|\psi_0\rangle = \sum_k \lambda_{m,\tau}(k,k+G)(n-(v+4))\,|\psi_0\rangle = 0$, when $n-(v+4)=0$

Raising operators within $\mathrm{U}(4)$ applying on ground states are also ground states

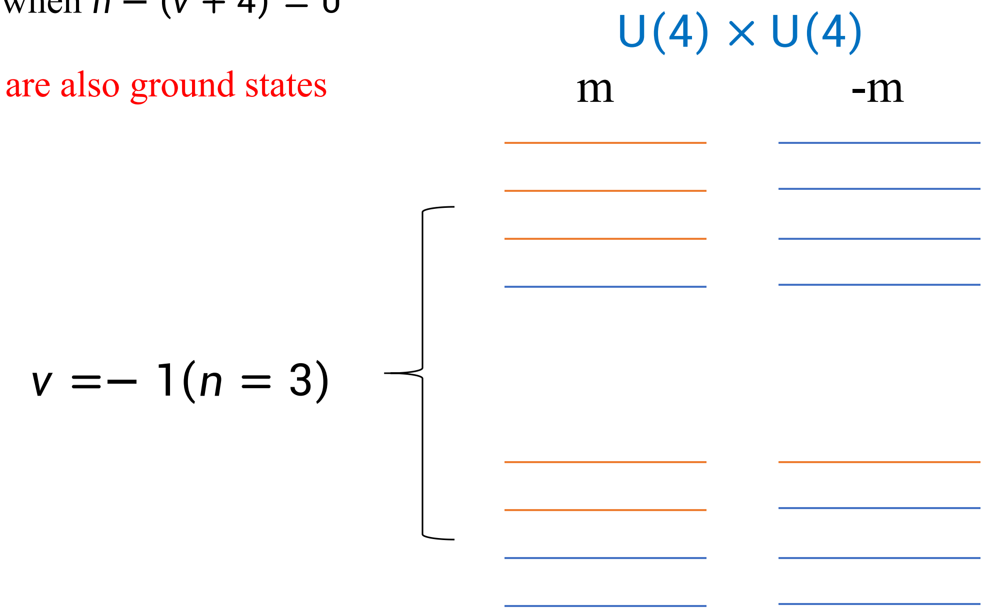
$H_I\Delta^\dagger_{m,\sigma,\sigma'}|\psi_0\rangle = \Delta^\dagger_{\sigma,\sigma'}H_I|\psi_0\rangle = 0$

$\Delta^\dagger_{m,\sigma,\sigma'} \equiv \sum_k c^\dagger_{k,m,\sigma}c_{k,m,\sigma'}$



$\sigma,\ \sigma'$ for empty and occupied

spin-valley $\mathrm{U}(4)$ in Chern sector m.



TBG in other integer fillings

Ground state degeneracy by SU(4) Young diagram

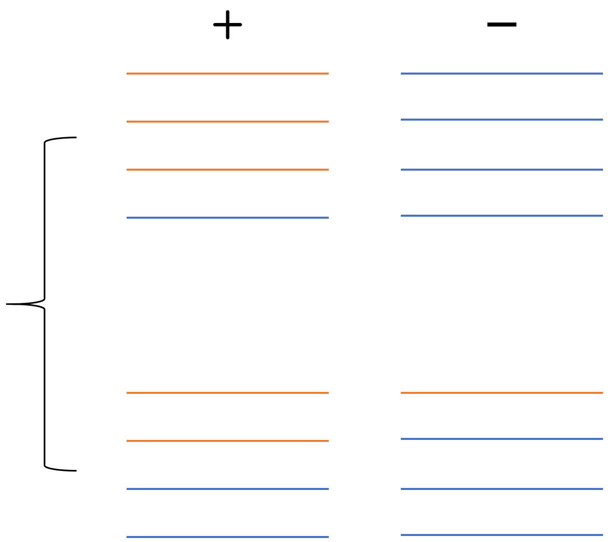
$\mathrm{U}(4) \times \mathrm{U}(4)$

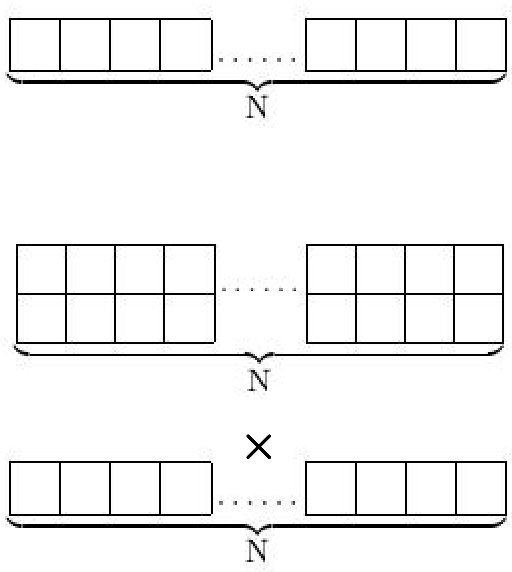
Young diagram

Degeneracy

Chern number

$\nu = -1 (n = 3)$





$$\frac{(N+3)(N+2)(N+1)}{3!}$$

$C = 3$

$$\frac{(N+3)^2(N+2)^3(N+1)^2}{3!\,3!\,2!}$$

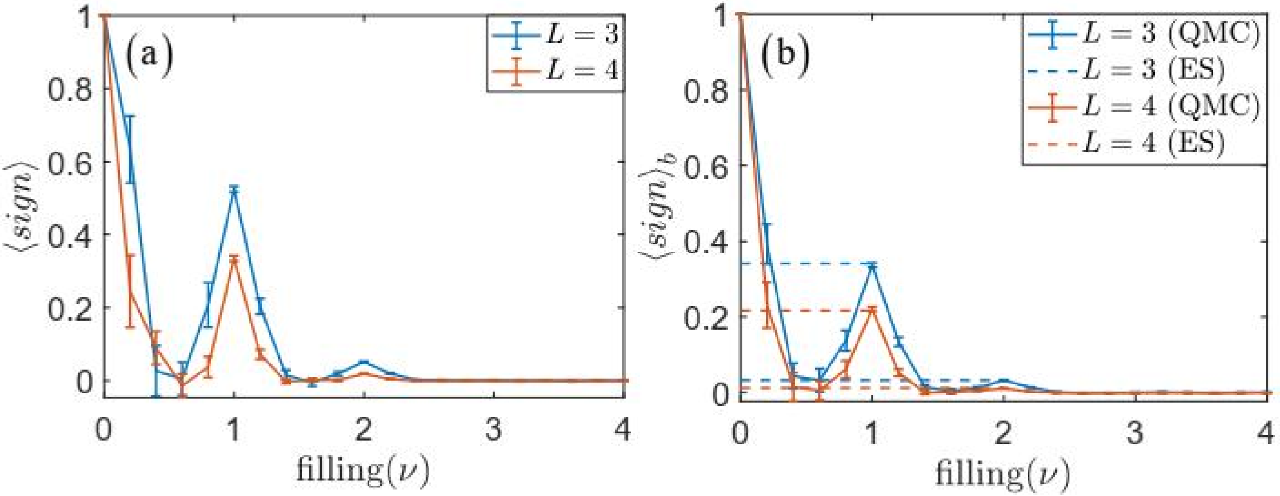
$C = 1$ ✓

TBG in other integer fillings

Polynomial sign bounds behavior at low temperature

$$\langle sign\rangle \geq \frac{g_{v=1}}{g_{v=0}} = \frac{\frac{(N+3)^2(N+2)^3(N+1)^2}{3!\,3!} + \frac{(N+3)(N+2)(N+1)}{3}}{\frac{(N+3)^2(N+2)^4(N+1)^2}{3!\,3!\,2!\,2!} + \frac{(N+3)^2(N+2)^2(N+1)^2}{3!\,3} + 2} \propto N^{-1}$$

Filling(ν)	Chiral($\gamma = 0$)
0	1
± 1	N^{-1}
± 2	N^{-2}
± 3	N^{-5}
± 4	N^{-8}



Corollary II: For a Hamiltonian like

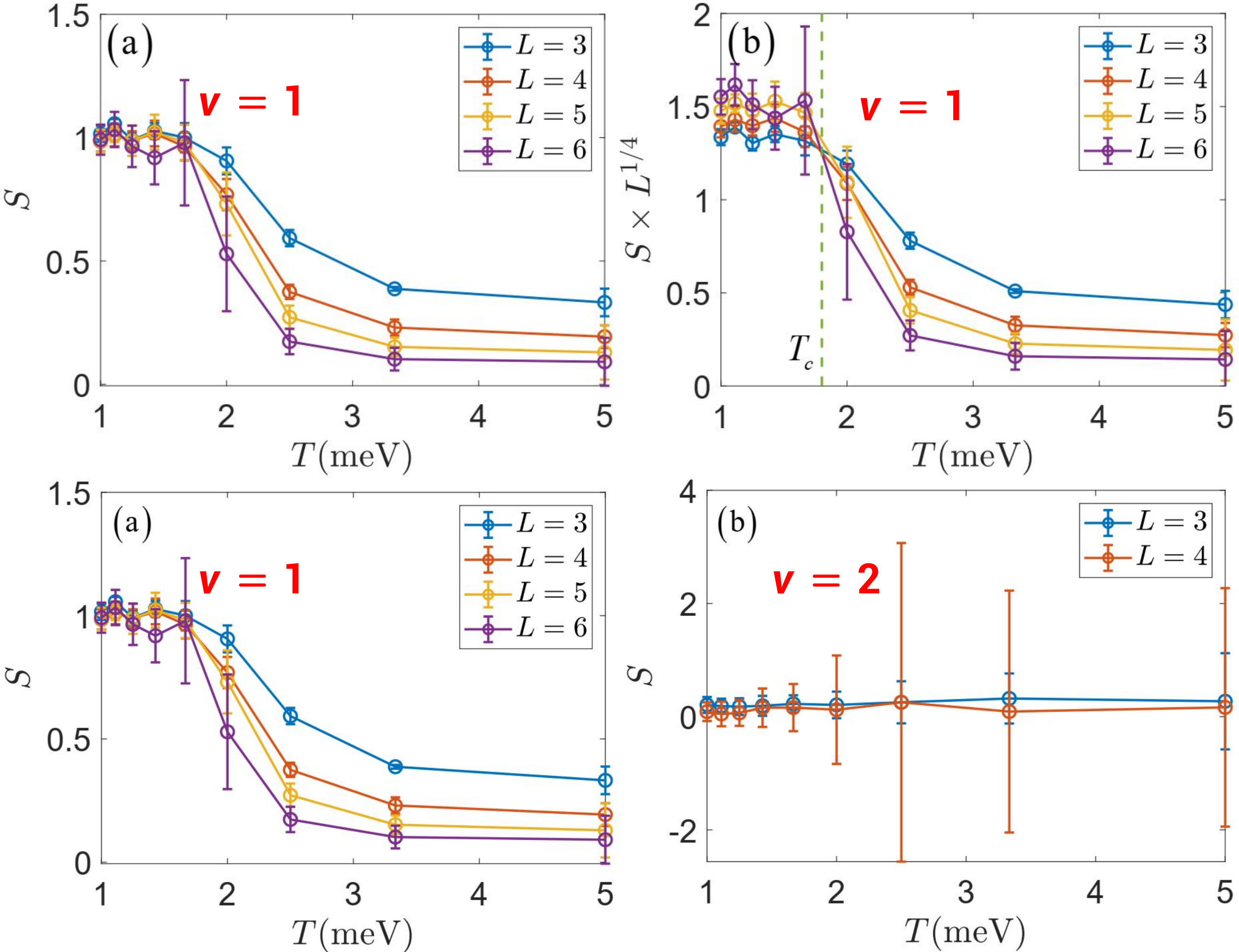
$$H = K + \sum_A (A - \mu_A)^2$$

where A and K are fermion bilinears and μ_A is real constant number. If for a certain group of μ_A, there is no sign problem, one can take $Z_{|D|}$ as a reference system (This can be seen by noticing μ_A only contributes a phase in D).

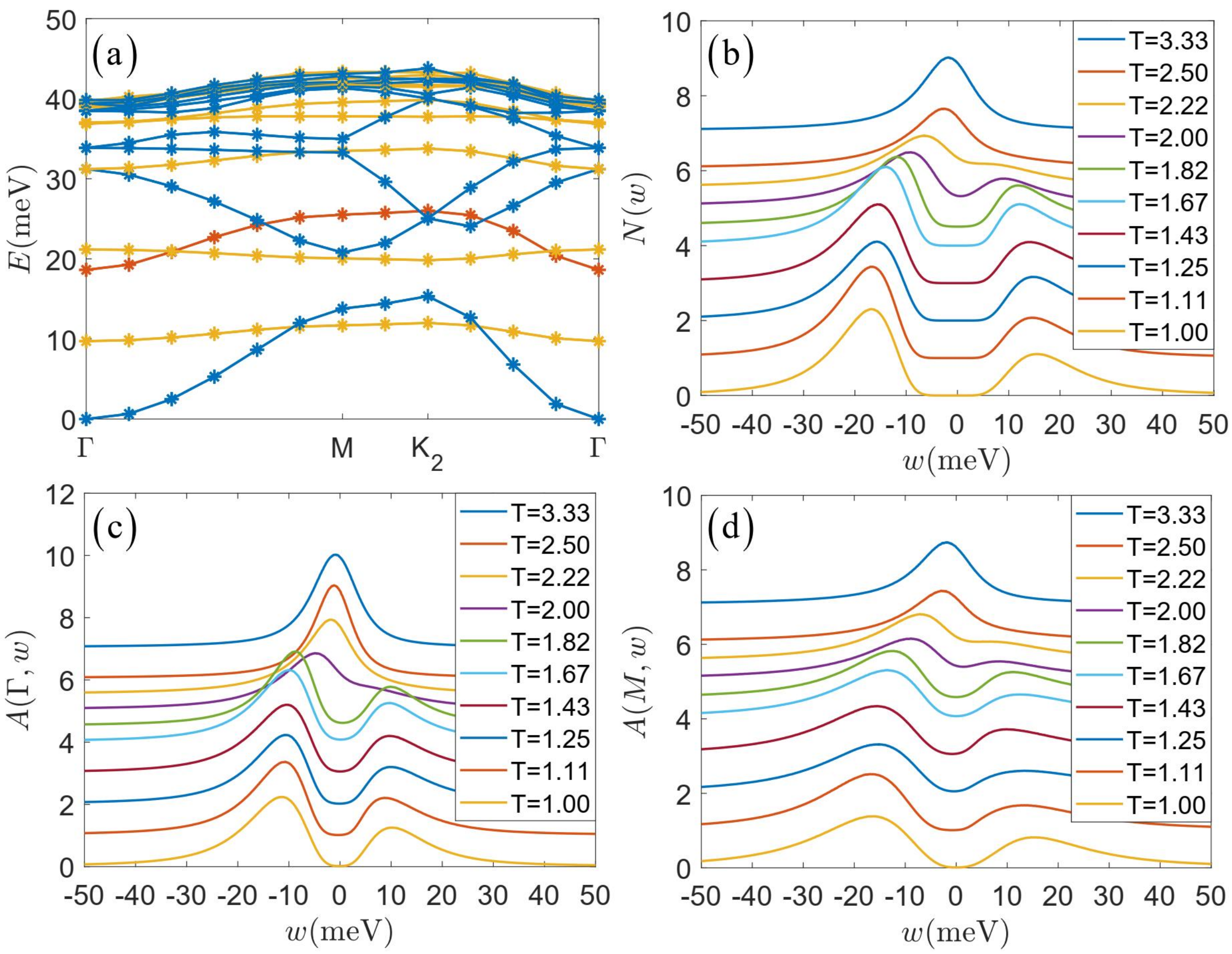
$$\langle sign\rangle \geq \frac{g_D e^{-\beta(E_D - E_{|D|})}}{g_{|D|}}$$

TBG in other integer fillings

Finite temperature topological phase transition



$v = 1$



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Thanks