Sign Problem Finds Its Bounds

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Sign problem in quantum Monte Carlo (QMC) simulation appears to be an extremely hard problem. Traditional lore passing around for years tells people that when there is a sign problem, the average sign in QMC simulation approaches zero exponentially fast with the space-time volume of the configurational space. We, however, show this is not always the case and manage to find bounds for the sign problem. Our new understanding is based on a direct connection between the sign problem bounds and ground state properties on finite size and could distinguish when the bounds have the usual exponential scaling, and when they are bestowed on an algebraic scaling. We show such algebraic sign problems in fermionic QMC for quantum Moiré lattice models both in real and momentum space at low temperature limit. Our approach inspires new ways to cure, ease and even make use of the sign problem.

Introduction.- Quantum Monte Carlo (QMC) is a standard and unbiased method for studying strongly correlated systems, widely used in condensed matter, high energy and quantum material research [1–4]. In QMC, the partition function of a many-body system is cast into a sum (or integral) over configurations in a chosen basis, and the important sampling scheme could in principle cover the exponentially large configurational space in polynomial time. However, in reality, very often due to inadequate choices of basis, QMC simulations suffer from the so-called sign problem [5], in which configurational weights become negative or even complex and can no longer be interpreted as classical probabilities. It has been proven that if the nondeterministic polynomial (NP) hard problem can be solved efficiently, then the obtained scheme can be used to solve the sign problem [6], so that many interesting and fundamental questions in quantum many-body systems will be understood thereafter. Unfortunately, this has not happened yet.

This does not mean the sign problem itself is NP hard and cannot be cured. In fact, there are cases the sign problem can be cured by choosing new bases where certain symmetries or mathematical operations, such as time reversal or anti-unitary symmetry [7–10], meron cluster [11], Fermi bags [12], split-orthogonal group [13], Majorana time-reversal symmetry [14–16], Majorana positivity [17], semigroup approach [18] and pseudo-unitary group [19], can be used to prove the simulation is sign problem free. In some other cases, sign problem can be alleviated by an optimal choice of basis [20–34], or through adiabatic method [35].

The great efforts to avoid or alleviate sign problem are encouraging, though successful cases are quite limited and the understanding of the origin of the sign problem is still at a case by case stage. For example, frustrated spin systems often have a sign problem because off-diagonal operators in spin Hamiltonian bring a negative matrix element [36, 37]. While in fermionic systems, negative weights usually arise from the Pauli exclusion principle [6] or improper choice of the Hubbard-Stratonovich (HS) decoupling scheme [38]. There also exists suggestion that the negative sign of a configuration is a topological invariant, which is an imaginary time counterpart of the Aharonov-Anandan phase and can be reduced to a Berry phase in the adiabatic limit [39]. Moreover, it was shown recently that some interacting models may have intrinsic sign problem, which cannot be cured regardless [40–43], and the sign problem has even been linked to quantum phase transitions [44–46].

However, in general, the situation is not completely optimistic and a universal guiding principle to cure, ease and even make use of the sign problem is still missing. It is generally believed that if there is a sign problem in QMC simulation, then the average sign will scale exponentially fast to zero with the space-time volume. But in our recent attempts of model design and QMC solution for quantum moiré lattice models at integer filling, both for real [47] and momentum space [48], interesting outliers, where the average sign scales algebraically with system size and is independent with temperature at low temperature limit, were discovered. These results challenge the conventional thoughts and urge a new understanding on universal properties of sign problem.

In this Letter, we offer such a new understanding by unveiling a sign bounds theory that connects the sign problem at low temperature limit with ground state properties of the system at hand, i.e., ground state energy (GSE) and ground state degeneracy (GSD) in finite size system. The bounds calculation requires an estimation for GSE and GSD of the original system and a refer-
ence system. When applied to specific models, it can distinguish situations where the average sign bounds is exponential and where it is algebraic. Then, we apply our theory to understand the algebraic scaling of average sign in a class of positive semidefinite Hamiltonians which have immediate relevance to the on-going efforts in understanding the experimental discoveries of correlated insulators and superconductors in the quantum moiré materials [47, 49–52].

Sign bounds theory.- For a generic quantum many-body system with Hamiltonian $H$, partition function $Z$, GSE $E$ and GSD $g$, we have the relation $Z = \text{Tr}[e^{-\beta H}] = g \cdot e^{-\beta E}$ at low temperature limit $\beta \equiv 1/T \to \infty$ for a finite size system. Then, in the setting of ferimonic QMC, the partition function is further written as the weighted average of fermion determinants after the Trotter decomposition and HS transformation, $Z_D = \sum_{\{l\}} P(\{l\}) D(\{l\}) \equiv (D)$, where $l$ represents different configurations, $P(\{l\})$ is the configurational weight for determinant $D(\{l\})$ (see Sec.1 in Supplementary Materials (SM) [53] for details). Since we only consider Hermitian system by default, $Z_D = \Re\{Z_D\} = \langle \Re(D) \rangle$. Now, consider a reference system with the same configuration space, but with non-negative determinant $V(\{\bar{l}\}) \geq 0$ for any configuration $\bar{l}$, where $\langle V \rangle \equiv \sum_{\bar{l}} P(\{\bar{l}\}) V(\{\bar{l}\})$ corresponds to a partition function $Z_{\bar{l}}$ of a physical Hamiltonian with explicit fermion interactions. Then we can define the average sign bounds on the reference system $V$ at low temperature limit as $\langle \text{sign}\rangle_{V}$

\[
\langle \text{sign}\rangle_{V} = \frac{Z_D}{Z_{\bar{l}}} = g_D e^{-\beta E_D} g_{\bar{l}} e^{-\beta E_{\bar{l}}}. \tag{1}
\]

While in simulation we usually take average sign $\langle \text{sign}\rangle = \frac{\langle \Re(D) \rangle}{\langle \Re(D) \rangle}$ where it is hard to find a physical partition function $Z_{\langle \Re(D) \rangle}$ corresponding to $\langle \Re(D) \rangle$, we can give a boundary behavior by discussing $\langle \text{sign}\rangle_{V}$ where reference system can be $Z_{D[D], Z_{\bar{l}[D]}, \text{etc.}}$. According to the principle of weighted average, we have $\langle \Re(D) \rangle \leq \langle \Re(D) \rangle \leq \sqrt{\langle D \rangle^2}$ and $\langle \Re(D) \rangle \leq \langle \Re(D) \rangle \leq \langle D \rangle$, which implies

\[
\frac{g_D e^{-\beta E_D}}{\sqrt{g_{\bar{l}} e^{-\beta E_{\bar{l}}}}} \leq \langle \text{sign}\rangle \leq 1
\]

\[
\frac{g_D e^{-\beta E_D}}{g_{\bar{l}} e^{-\beta E_{\bar{l}}}} \leq \langle \text{sign}\rangle \leq 1 \tag{2}
\]

corresponding to reference system $Z_{\{D\}}$ or $Z_{\{D\}}$ at the low temperature limit respectively.

The discussions above give rise to three immediate consequences: (1) When $E_D = E_V$, the explicit exponential dependence of the average sign on system size is gone, with only the dependence on GSD between original and reference systems, which usually only scales at most polynomially with spatial system size. (2) When $E_D \neq E_V$, an exponential dependence of the average sign bounds on system size is expected. Little constraint about average sign is given by this reference system. But select a better reference system making $E_V$ closer to $E_D$ has a chance to improve the bounds. (3) Based on finite size scaling of the average sign and the calculation of GSE and GSD for reference systems, properties of GSE and GSD for original system may be extracted.

Algebraic scaling of average sign.- An important application of above sign bounds theory is to understand algebraic scaling of average sign we found [47, 48]. Our discoveries are made in the process of model design and computational solution for understanding the rich phenomena of quantum moiré materials, in particular the correlated insulators and superconducting phases in twisted bilayer graphene and transition metal dichalcogenides. These 2D quantum materials with flat band and long-range Coulomb interaction have stimulated us to study the real space extended Hubbard models [47, 54–57], as well as invent the momentum space QMC method to solve interacting models with truly long-range Coulomb [49, 51, 52]. Although most simulations till now are focused at the charge neutrality point [47, 49, 51, 54–57], we come to the realization that many related models in flat band systems acquire a positive semidefinite (PSD) Hamiltonian, as discussed in earlier analytic works [58–61]. We find out PSD Hamiltonian has a different sign behavior, which in many cases the average sign scales polynomially with the system sizes and to a finite constant with lowering temperature both in the real space model [47] and in the momentum space model [48]. Such polynomial sign problem makes the large-scale QMC simulation very applicable in flat band quantum moiré lattice models.

Below we discuss the algebraic scaling of the average sign bounds according to our theory and structure the corresponding systems within two corollaries.

Corollary I.- For a fermion Hamiltonian whose sign of QMC for every configuration is real, we can introduce another $U(2)$ freedom $s \in \{+, -\}$ such as spin or valley, to prepare a reference system with GSE $E_{\{D\}}$ and GSD $g_{\{D\}}$. Then for the original system, $\langle \text{sign}\rangle \geq g_D e^{-\beta (E_D - E_{\{D\}}/2)} / \sqrt{g_{\{D\}}^2}$. If $E_D = E_{\{D\}}/2$, $\langle \text{sign}\rangle \geq g_D / \sqrt{g_{\{D\}}^2}$.

Examples.- We introduce two cases here, which are set in momentum space, with a generic PSD Hamiltonian (e.g., describing the long-range Coulomb interaction in flat band system)

\[
H = \sum_{q \neq 0} V(q) \rho_{-q} \rho_q = \sum_{q \neq 0} V(q) \rho_0^q \rho_q \tag{3}
\]

where $\rho_q = \sum_{i,j} \left( \lambda_{i,j}(q) e_i^\dagger c_j - \frac{1}{2} \mu_q \right)$, $i,j$ are matrix indexes with dimension $N$ (e.g., the momentum grid in moiré Brillouin zone, $N = 6 \times 6, 9 \times 9, \cdots$), and the averagely half-filled physical system requires $\langle V(q) \rangle = V(-q) > 0$, $\text{Tr}(\lambda_{i,j}(q)) = \mu_q$. In our previous momentum space QMC work [19], we proved that $\text{Tr}(\lambda_{i,j}(q)) = \mu_q$.
guarantees the sign for every configuration is real. Then one can require zero-energy ground state for observing \(\langle \text{sign} \rangle \geq g_D/\sqrt{|g_D|^2}\) behavior.

In our case 1, \(\mu_q = 0\) and \(\lambda_{i,j}(q)\) is set randomly. For \(\mu_q = 0\), one can easily check empty and full states are two ground states with zero energy. Random \(\lambda_{i,j}(q)\) means there should be no other symmetry so that no other degeneracy. Then we have \(g_D = 2\). After we introduce another freedom \(s \in \{+, -\}\), which means now \(\rho_{s,q} = \sum_i \lambda_{i,j}(q) \cdot (c^\dagger_{i,j}c_j + c^\dagger_{i,-j}c_{-j}) - \mu_q\). For computing degeneracy \(g_{D^2}\), one can define a raising operator

\[
\Delta^\dagger = \sum_{j'} c^\dagger_{j',+}c^\dagger_{j',-}.
\]

By noticing \([\Delta^\dagger, \rho_{s,q}] = 0\) and \(|\psi_{+,empty}\rangle \otimes |\psi_{-,full}\rangle\) is a ground state. We can apply \(\Delta^\dagger\) at most \(N\) times on this state, and this gives us \(N + 1\) ground states with \(N\) particles. Besides, we also have ground states with \(0\) and \(2N\) particles (i.e. \(|\psi_{+,empty}\rangle \otimes |\psi_{-,empty}\rangle\) and \(|\psi_{-,full}\rangle \otimes |\psi_{-,full}\rangle\)). Together, \(g_{D^2} = N + 3\) for random \(\lambda_{i,j}(q)\) so that \(\langle \text{sign} \rangle \geq g_D/\sqrt{|g_D|^2} = 2/\sqrt{N + 3}\). This means at low temperature and large size limit, \(\langle \text{sign} \rangle\) will not decay faster than \(N^{-\frac{1}{2}}\).

In our case 2, \(\mu_q \neq 0\) and there are two band labels \(m, n \in \{1, -1\}\) for \(\lambda_{i,j,m,n}(q) = m \cdot n \cdot \lambda_{i,j,m,n}(q)\) (e.g., chiral flat band limit for spin-polarized and valley-polarized TBG at half filling, following gauge chosen in Ref. [59][60]). Now \(\rho_q = \sum_{i,j,m,n} (\lambda_{i,j,m,n}(q)c^\dagger_{i,m}c_{j,n} - \frac{1}{2}\mu_q)\) and there are two degenerate ground states with Chern number \(\pm 1\), i.e. \(g_D = 2\). Again, after introducing freedom \(s \in \{+, -\}\), \(\rho_{s,q} = \sum_{i,j,m,n} (\lambda_{i,j,m,n}(q) \cdot (c^\dagger_{i,m}c_{j,n} + c^\dagger_{i,-m}c_{-j,-n}) - \mu_q)\).

One can define two raising operators (see Sec.II in SM [53])

\[
\Delta_1^\dagger = \sum_j (c^\dagger_{j',1,+} + ic^\dagger_{j',1,-})(c_{j',1,-} - ic_{j',1,+})
\]

\[
\Delta_2^\dagger = \sum_j (c^\dagger_{j',1,+} - ic^\dagger_{j',1,-})(c_{j',1,-} + ic_{j',1,+})
\]

Here \(i\) is the imaginary unit. It is straightforward to verify \([\Delta_1^\dagger, \rho_{s,q}] = [\Delta_2^\dagger, \rho_{s,q}] = 0\) and \([\Delta_1^\dagger, \Delta_2^\dagger] = [\Delta_1^\dagger, \Delta_2^\dagger] = 0\). This means \(\Delta_1^\dagger\) and \(\Delta_2^\dagger\) generate two groups of orthogonal eigenstates with the same energy. By noticing \(|\psi_{+,empty}\rangle \otimes |\psi_{-,full}\rangle\) is a ground state, apply \(\Delta_1^\dagger\) or \(\Delta_2^\dagger\) independently will give \((N + 1)^2\) orthogonal zero-energy states with zero Chern number. Here \(N\) is dimension of label \(i, j\) in \(\lambda_{i,j,m,n}(q)\). Besides, there are also two states with non-zero Chern number, on which raising operators apply are equal to \(0\) so that no other states will be given, \(g_{D^2} = (N + 1)^2 + 2\). This means for this model, \(\langle \text{sign} \rangle \geq 2/(\sqrt{(N + 1)^2} + 2\) as shown in Fig. 1(b).

Corollary II.- For a Hamiltonian with a PSD interaction part \(\sum\alpha(A - \mu)^2\) and a kinetic part \(K\), where \(A\) and \(K\) are the fermion bilinears and \(\mu\) is the chemical potential. If for a certain \(\mu\), there is no sign problem, then at low temperature limit, average sign bounds for different \(\mu\) behave differently according to GSE and GSD for reference system \(Z_{D^2}\) which corresponds to partition function of sign problem free filling. This can be seen by noticing \(\mu\) only contributes a phase in \(D\{\{\}\}\) (see Sec.I in SM [53]). Generally, \(\langle \text{sign} \rangle \geq g_{D^2}e^{-\beta(E_D - \beta E_{D^2})}/g_{D^2}\). If \(E_D = E_{D^2}\), \(\langle \text{sign} \rangle \geq g_D/g_D\).

Example.- It is easy to notice this corollary can give an average sign bounds behavior at low temperature limit in repulsive Hubbard model, where the usual exponential decay of average sign is commonly seen. Though QMC may say little about \(E_D\) and \(g_D\), one could expect with

FIG. 1. For three example cases, the average sign bounds, allowed region, QMC measurement \(\langle \text{sign} \rangle\) and its polynomial fitting with fitting lines are shown. The errorbars in QMC data are smaller than the symbol size. (a) For momentum space 1 model, bounds are determined by \(\langle \text{sign} \rangle \geq 2/\sqrt{N + 3}\). QMC measurements for \(N = 18, 32, 50, 72, 98, 128, 162\) are carried out at a (sign) converged temperature. Fitting line \(\propto N^{-0.23}\). (b) For momentum space 2 model, bounds is determined by \(\langle \text{sign} \rangle \geq 2/(N + 2)\) and \(N = 18, 72, 162, 288, 450, 648, 882\) are measured from QMC [27]. Fitting line \(\propto N^{-0.98}\).
the improvement of constrained path QMC, density matrix renormalization group and tensor-network type methods, GSE and GSD for finite size doped Hubbard system can be obtained [52] [63], so that theoretical sign bounds behavior $g_{DE}e^{-\beta|E_D-E_D|}/|g|_{DE}$ can be achieved. Since there have been many discussions on the sign problem therein [5] [43] [64] [68], here we still focus the application of this corollary on a PSD Hamiltonian without kinetic part $K$. We study the Kang-Vafek’s real space model [58] for twisted bilayer graphene at flat band limit with 1/4 or 3/4 filling ($\nu = \pm 2$), whose GSE $E = 0$ is equal to that at half filling ($\nu = 0$). This example gives an explanation for algebraic average sign observed in Ref. [47].

The model is written below

$$H = U \sum_{O} (Q_{O} + \alpha T_{O} - \nu)^2$$

where $Q_{O} = \frac{1}{3} \sum_{\sigma, \tau} \sum_{l=1}^{6} c_{R+l, \sigma, \tau}^\dagger c_{R+l, \sigma, \tau} - 4$, $T_{O} = \sum_{\sigma, \tau} \sum_{l=1}^{6} (-1)^l c_{R+l, \sigma, \tau}^\dagger c_{R+l, \sigma, \tau} + h.c.$, $\nu$ is used to control filling, $\sigma, \tau$ are spin and valley indexes, $R + \delta_l$ represents site $l$ in a single $R$ hexagon and $U, \alpha$ are real constants. Attention to the subtraction of a constant $4$ in the definition of operator $Q_{O}$ which moves the charge neutrality point to $\nu = 0$. We consider the infinite-$U$ case as studied in Ref. [47]. Fixing $\alpha$, then the only parameter is $\beta U$, and any finite $\beta$ in the infinite-$U$ limit corresponds to low temperature limit. We consider the system with linear system size $L$ up to $L = 21$ and total number of sites is $N = 2L^2$. This model is sign problem free at charge neutrality [50] [57], with partition function identical to $Z_{|D|}$, as when $\nu$ is away from charge neutrality, it only introduce a phase to the weight [53]. As the real space model is PSD, and one can construct zero energy ground state both at charge neutrality and at $\nu = \pm 2$ with GSD $g_D = (N + 3)(N + 2)(N + 1)/6$ for $\nu = \pm 2$ [58] [60] and GSD $g_{|D|} = (N + 3)(N + 2)^2(N + 1)/12$ for $\nu = 0$ [53] [60] (see Sec. III in SM [53] for the Tensor Young tableau method in which the GSD are obtained), therefore $\langle \text{sign} \rangle \geq g_{D}/g_{|D|} = 2/(N + 2)$. Fig. 1(c) shows the average sign presented in Ref. [47], comparing with the average sign bounds we proposed.

**Conclusion and Discussion.**— Our sign bounds theory builds a direct connection between the sign problem at low temperature limit and properties of ground state on finite size quantum many-body systems. The average sign bounds depends on GSE and GSD of the original system and the reference system as shown in Eqs. (1) and (2). Based on these general observations, we further derive two corollaries, which are used to understand the average sign bounds changing with filling and demonstrate the algebraic scaling of average sign in a class of PSD models which have immediate relevance towards the quantum morié materials.

Our idea can also be extended to projection version of QMC as well. Suppose we have a trial wavefunction with $|\Psi_T \rangle = \sum c_{n} |\Psi_n \rangle$ where $|\Psi_n \rangle$ is the eigenstate of $H$ with eigenvalue $E_n$. In the projection version of QMC, the true wavefunction is achieved by projection, i.e., $|\Psi_0 \rangle \sim \lim_{\theta \to 0} e^{-\theta H} |\Psi_T \rangle$. To keep similar notation with finite temperature case, we denote $Z_D = \langle \Psi_T | e^{-g_{DE} H} | \Psi_T \rangle = c_{DE} e^{-2\Theta E_D}$, where $c_{DE} = \sum_{n \in \mathbb{D}} |c_n|^2$ is the ground state component in $|\Psi_T \rangle$ and $E_D$ is the GSE. For reference system, we have $e^{\nu} = c_{DE} e^{-2\Theta E_D}$, where $c_{DE}$ is the reference system ground state component in $|\Psi_T \rangle$ and $E_D$ is the reference system GSE. Then the average sign bounds is

$$\langle \text{sign} \rangle_\nu = \frac{c_{DE} e^{-2\Theta E_D}}{c_{DE} e^{-2\Theta E_D}}.$$

This implies to alleviate the sign problem, it is important to make the trial wavefunction have larger components of the ground state and make the reference system have closer GSE with origin system. This may explain the recent proposed adiabatic method, where the trial wavefunction is adiabatically improved and the closeness of reference GSE is well expected [35].

In a similar spirit, with the further improvement of DMRG and tensor-network type of approaches, where the low temperature, GSE and GSD on finite size systems are expected to be obtained with better accuracy, it will be natural to make use of these information and perform the analysis with our theory to provide (hopefully improved) bounds of QMC on the systems with conventional exponential sign problem, such as doped Hubbard model or quantum spin systems with frustration. It encourages to add a constant to the Hamiltonian to minimize the GSE difference between $E_D$ and $E_V$, such that a reducing of the sign problem is expected. It reminds the crucial constant term used in continuous-time QMC simulations [64]. Moreover, as our theorem directly relates the sign problem to the physical properties of the system, it implies there may be important information hidden inside configurations even when the simulation has sign problem. Therefore, machine learning and related data mining of Monte Carlo data with sign problem are encouraging [69]. Based on a careful scaling analysis of the average sign, a calculation of the GSE and GSD of reference systems, properties of the GSE and GSD of original systems can also be extracted.

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The determinant quantum Monte Carlo algorithm and...
SUPPLEMENTAL MATERIAL FOR SIGN PROBLEM FINDS ITS BOUNDS

Section I: Determinant QMC algorithm and sign problem

Here we introduce how determinant QMC works both for momentum cases and real space case. We follow the implementation of momentum space quantum Monte Carlo developed by us in Ref. [59].

\[
H = \sum_{q \neq 0} V(q) \rho_q \rho_{-q}
\]

\[
\rho_q = \sum_{i,j,m,n} \left( \lambda_{i,j,m,n}(q) c^\dagger_{i,m} c_{j,n} - \frac{1}{2} \mu_q \right)
\]

(8)

According to the discrete Hubbard-Stratonovich (HS) transformation, \( e^{\alpha O^2} = \frac{1}{2} \sum_{l=\pm 1, \pm 2} \gamma(l) e^{\sqrt{\alpha} \eta(l)^2} + O(\alpha^4) \), where \( \gamma(\pm 1) = 1 + \sqrt{3} \), \( \gamma(\pm 2) = 1 - \sqrt{3} \), \( \eta(\pm 1) = \pm \sqrt{2(3 + \sqrt{6})} \) and \( \eta(\pm 2) = \pm \sqrt{2(3 - \sqrt{6})} \), we can rewrite the partition function as,

\[
Z = \text{Tr} \left\{ \prod_{\tau} e^{-\Delta \tau H(\tau)} \right\} = \text{Tr} \left\{ \prod_{\tau} e^{-\Delta \tau \sum_{q \neq 0} \frac{\nu(q)}{2} (\rho_{q} + \rho_{-q})^2 - (\rho_{q} - \rho_{-q})^2) \right\}
\]

\[
\approx \sum_{\{ l_q, \tau \}} \prod_{q \neq 0} \frac{1}{16} \gamma(l_{q,1,\tau}) \gamma(l_{q,2,\tau}) \text{Tr} \left[ \prod_{\tau} \prod_{q \neq 0} e^{i\eta(l_{q,1,\tau})} A_q (\rho_{q} + \rho_{-q}) e^{\eta(l_{q,2,\tau})} A_q (\rho_{q} - \rho_{-q}) \right] \]

(9)

Here \( \tau \) is the imaginary time index with step \( \Delta \tau \), \( A_q = \sqrt{\Delta \tau \nu(q)} \) and \( \{ l_{q,1,\tau}, l_{q,2,\tau} \} \) are the four-component auxiliary fields. By defining \( P(\{ l_q, \tau \}) \equiv \prod_{q \neq 0} \gamma(l_{q,1,\tau}) \gamma(l_{q,2,\tau}) \) and \( D(\{ l_q, \tau \}) \equiv \text{Tr} \left[ \prod_{\tau} \prod_{q \neq 0} e^{i\eta(l_{q,1,\tau})} A_q (\rho_{q} + \rho_{-q}) e^{\eta(l_{q,2,\tau})} A_q (\rho_{q} - \rho_{-q}) \right] \)

one can see partition function \( Z \) as sample average for \( D(\{ l_q, \tau \}) \) with configuration weight \( P(\{ l_q, \tau \}) \) (i.e., \( Z = \sum_{\tau, \{ l_q \}} P(\{ l_q, \tau \}) D(\{ l_q, \tau \}) \)). Since \( P(\{ l_q, \tau \}) \) here comes from continuous HS transformation coefficient (i.e., \( \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2} x^2} \) in \( e^{\alpha O^2} = \frac{1}{\sqrt{2\pi}} \int e^{-\frac{1}{2} x^2} e^{\sqrt{\alpha} \eta(x)} dx \)), it has already been normalized and only depends on configuration.

For corollary II, the decouple routine is similar. Since it is straightforward to see \( \mu_q \) in \( D(\{ l_q, \tau \}) \) is only shown in \( e^{i\eta(l_{q,1,\tau})} \mu_q \) form, different filling with different \( \mu_q \) must have the same \( |D(\{ l_q, \tau \})| \). If for a filling where the weight for any configuration is non-negative, \( D(\{ l_q, \tau \}) \) for this filling is equal to \( |D(\{ l_q, \tau \})| \). This is why a reference system \( Z_{|D|^2} \) can work. Besides, if \( D(\{ l_q, \tau \}) \) for any configuration is real, since \( |D|^2 = D^2 \), generally a reference system \( Z_{|D|^2} \) can work by introducing another \( U(2) \) freedom as shown in corollary I.

Ensemble average of any observables \( \hat{O} \) can be written as,

\[
\langle \hat{O} \rangle = \frac{\text{Tr} \left\{ \hat{O} e^{-\beta H} \right\}}{\text{Tr} \left\{ e^{-\beta H} \right\}} = \frac{\sum_{\{ l_q, \tau \}} P(\{ l_q, \tau \}) \text{Tr} \left[ \prod_{\tau} \hat{B}_\tau(\{ l_q, \tau \}) \right]}{\sum_{\{ l_q, \tau \}} P(\{ l_q, \tau \}) \text{Tr} \left[ \prod_{\tau} \hat{B}_\tau(\{ l_q, \tau \}) \right]}
\]

(10)

Here \( \hat{B}_\tau(\{ l_q, \tau \}) = \prod_{\tau \neq 0} e^{i\eta(l_{q,1,\tau})} A_{\tau} (\rho_{\tau} + \rho_{-\tau}) e^{i\eta(l_{q,2,\tau})} A_{\tau} (\rho_{\tau} - \rho_{-\tau}) \). Now, we see \( P_1 = P(\{ l_q, \tau \}) \text{Tr} \left[ \prod_{\tau} \hat{B}_\tau(\{ l_q, \tau \}) \right] \) as possibility weight and \( \langle \hat{O} \rangle = \frac{\text{Tr} \left[ \hat{O} \prod_{\tau} \hat{B}_\tau(\{ l_q, \tau \}) \right]}{\text{Tr} \left[ \prod_{\tau} \hat{B}_\tau(\{ l_q, \tau \}) \right]} \) as sample value for configuration \( \{ l_q, \tau \} \). Then Markov chain Mento Carlo can compute this \( \langle \hat{O} \rangle \). That is how determinant QMC works in sign problem free case (i.e., \( P_1 \) is real and \( P_1 \gg 0 \) for all configurations). But this is not the case at most of time. With sign problem, one can still simulate according to QMC by reweighting [5].
(\hat{O}) = \frac{\sum_i P_i \langle \hat{O} \rangle_i}{\sum_i P_i} = \frac{\sum_i |R(P_i)\rangle_i \langle \hat{O} |R(P_i)\rangle_i}{\sum_i |R(P_i)\rangle_i \langle \hat{R}(P_i) |} = \frac{\langle \hat{O} |R(P_i)\rangle}{\langle \text{sign} | \rangle}

One can see $|R(P_i)\rangle$ as a well-defined possibility weight and $\langle \hat{O} |R(P_i)\rangle$ is the measurement result according to this weight. The ratio $\sum_i \frac{P_i}{|R(P_i)\rangle}$ is the average sign $\langle \text{sign} | \rangle$ we keep talking about. One can see if $\langle \text{sign} |$ is exponentially small, fluctuation of computing $\langle \hat{O} |R(P_i)\rangle$ will be exponentially large, which causes so called sign problem.

Section II: Raising operator construction

Here we introduce the way we use to look for raising operators. First, for random $\lambda_{i,j}$, $\rho_q = \sum_{i,j} \left( \lambda_{i,j}(q) c_i^\dagger c_j - \frac{1}{2} \mu_q \right)$ and $\rho_{s,q} = \sum_{i,j} \left( \lambda_{i,j}(q) \cdot \left( c_{i,+} c_{j,+} + c_{i,-} c_{j,-} \right) - \mu_q \right)$. If we want to find a two-fermion operator $\Delta^\dagger$ commuting with $\rho_{s,q}$, we only need to find a matrix commuting with $\rho_{s,q}$ in single-particle basis. The total dimension of $\rho_{s,q}$ can be written into $i,j$ space direct products $s \in \{+, -\}$ space noted by $K \otimes S$. Since generally $\lambda_{i,j}$ in $K$ space does not have any symmetry, one need a unit operator in this space to commute with $\rho_{s,q}$. While in $S$ space, one can see $\rho_{s,q,i,j}$ looks like

$$\rho_{s,q,i,j} = \begin{pmatrix} \lambda_{i,j}(q) & 0 \\ 0 & \lambda_{i,j}(q) \end{pmatrix}$$

which means actually any $2 \times 2$ matrix will commute with $\rho_{s,q,i,j}$. We choose a raising operator which makes charge flip from $- \to +$ space.

$$\Delta^\dagger_{i,j} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

Direct product those two parts of $\Delta^\dagger$, we achieve the raising operator we want

$$\Delta^\dagger = \sum_{i'} c_{i',+}^\dagger c_{i',-}$$

Then with similar spirit, we can derive $\Delta_{i,1}^\dagger$, $\Delta_{i,2}^\dagger$ in case 2. The only difference is now we have another band space $1, -1$. At chiral limit, $\rho_{s,q,i,j,+,,-}$ in band space looks like

$$\rho_{s,q,i,j,+,,-} = \begin{pmatrix} \lambda_{i,j,1,1}(q) & \lambda_{i,j,1,-1}(q) \\ -\lambda_{i,j,-1,1}(q) & \lambda_{i,j,-1,-1}(q) \end{pmatrix} = \lambda_{i,j,1,1}(q) \sigma_0 + i \lambda_{i,j,1,-1}(q) \sigma_y$$

Here $\sigma_0$ is a unit matrix and $\sigma_y$ is the Pauli matrix. For commuting with this matrix, the $2 \times 2$ matrix can be only in the form of $\alpha \sigma_0 + \beta \sigma_y$. For now, any choosing of $\alpha, \beta$ can generate one reasonable raising operator. If one also would like two different raising operators with different choosing of $\alpha, \beta$ satisfy $[\Delta_{i,1}^\dagger, \Delta_{i,2}^\dagger] = 0$, which means they are two groups of independent operators commuting with each other, $(\alpha_1 \sigma_0 + \beta_1 \sigma_y)(\alpha_2 \sigma_0 + \beta_2 \sigma_y) = 0$ must be satisfied. One simple choice is $(\sigma_0 + \sigma_y)(\sigma_0 - \sigma_y) = 0$. Then we achieve $\Delta_{i,1}^\dagger, \Delta_{i,2}^\dagger$ we used in the case 2 in the main text,

$$\Delta_{i,1}^\dagger = \sum_{j'} (c_{j',1,+} + ic_{j',1,-})(c_{j',1,-} - ic_{j',1,+}),$$
$$\Delta_{i,2}^\dagger = \sum_{j'} (c_{j',1,+} - ic_{j',1,-})(c_{j',1,-} + ic_{j',1,+}).$$

Section III: Tensor Young tableau method

For self consistency, we introduce another useful way, which is also used in Ref. [50, 60, 70], to compute the ground state degeneracy besides raising operator construction. This method works for models whose degeneracy are
introduced by SU(n) symmetry. \( g_D = (N+3)(N+2)(N+1)/6 \) for \( \nu = \pm 2 \) and GSD \( g_{|D|} = (N+3)(N+2)^2(N+1)/12 \) for \( \nu = 0 \) in Kang-Vafek’s real space model are calculated in this way.

In Kang-Vafek’s real space model case, degeneracy is introduced by SU(4) symmetry, where spin and valley contribute two SU(2). One can easily see any m-particle wave function can always be described by a 4-dimension rank-m tensor like \( T_{a_1,a_2,...,a_m} \), where different \( a_i \in \{1,2,3,4\} \) with 4 spin-valley dimensions label particles. SU(4) transformation for spin-valley space and \( S_m \) permutation for particle index are independent and will only change the tensor \( T \) to another tensor \( T' \) in the tensor space, which means \( T \) is well-defined for decomposition according to irreducible representation. By noticing the number of the same \( a_i \) must be less than lattice size \( N \), the Young diagram must have rows less than 4 and columns less than \( N \). The Young diagram to which full-filling one spin-valley flavor ground state for \( \nu = \pm 2 \) belongs is

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\begin{array}{ccccccc}
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\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
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\end{array}
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Assume only this irreducible representation contributes to ground states. Then counting the degeneracy is equal to count normal Young tableau of this Young diagram, which can be calculated by hook’s rule

\[
d_{[N]}(SU(4)) = \prod_j \frac{4 + j - 1}{j} \frac{(N+3)!}{N!} = \frac{(N + 3)(N + 2)(N + 1)}{6} \quad (17)
\]

While the Young diagram to which full-filling two spin-valley flavors ground state for \( \nu = 0 \) belongs is just

```
\begin{array}{ccccccc}
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
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\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\end{array}
```

The number of normal Young tableau calculated by hook’s rule is

\[
d_{[N,N]}(SU(4)) = \prod_{i,j} \frac{4 + j - i}{h_{i,j}} \frac{(N+3)!}{N!} \frac{(N+2)!}{2!} \frac{1}{(N+1)!} = \frac{(N + 3)(N + 2)^2(N + 1)}{12} \quad (18)
\]

It is worth to notice that there is also a numerical way to compute the GSD by QMC according to \( Z = \sum_{\{l\}} P(\{l\}) D(\{l\}) \). Our numerical results confirm the assumption that only one irreducible representation contributes to ground states in this case.