Majorana Positivity and the Fermion Sign Problem of Quantum Monte Carlo Simulations

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The sign problem is a major obstacle in quantum Monte Carlo simulations for many-body fermion systems. We examine this problem with a new perspective based on the Majorana reflection positivity and Majorana Kramers positivity. Two sufficient conditions are proven for the absence of the fermion sign problem. Our proof provides a unified description for all the interacting lattice fermion models previously known to be free of the sign problem based on the auxiliary field quantum Monte Carlo method. It also allows us to identify a number of new sign-problem-free interacting fermion models including, but not limited to, lattice fermion models with repulsive interactions but without particle-hole symmetry, and interacting topological insulators with spin-flip terms.

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Introduction.—A major difficulty in the study of strongly correlated systems is the exponentially large many-body Hilbert spaces, which are usually difficult to handle by analytic methods. Unbiased numerical methods are therefore indispensable. Among various numerical approaches, the quantum Monte Carlo (QMC) method can yield accurate results by taking stochastic but importance sampling over very small but representative portions of the many-body Hilbert space. An advantage of the QMC method is that it is scalable with the system size if there is no sign problem. Unfortunately, the sign problem exists in most interacting fermion and frustrated quantum spin systems.

The origin and manifestation of the sign problem vary in different QMC algorithms. A frequently used algorithm for lattice fermions is the auxiliary field determinantal method [1,2], in which the interaction terms are decoupled by the Hubbard-Stratonovich (HS) transformation into a superposition of quadratic fermion terms in the background of imaginary-time-dependent auxiliary fields. The fermion operators are then integrated out, yielding a fermion determinant that serves as the statistical weight for each HS field configuration. The sign problem emerges because this determinant is not always positive. In particular, the average value of the signs of these determinants often becomes exponentially small in the thermodynamic limit at low temperatures. This leads to uncontrollable statistical errors and ruins the QMC simulations. Although a great deal of effort has been made to solve, at least partially, this problem [3–12], a general solution is still lacking [13].

For certain classes of lattice fermion models, QMC simulations are proved to be sign-problem free. Familiar examples include the positive-U Hubbard model on a bipartite lattice at half filling [2], the negative-U Hubbard model [2,14], and their SU($2N$) generalizations [15–17]. The half-filled Kane-Mele-Hubbard model of interacting topological insulators is also sign-problem free [18,19]. For these models, after suitable HS decompositions with the Kramers time-reversal (TR) invariance [20,21], each determinant is factorized into a product of two complex conjugate determinants defined in two subspaces with opposite spins. A number of nonfactorizable models, such as the multicomponent and multiband Hubbard models [22–24], and the negative-U Hubbard models with spin-orbit coupling [25,26], can also be shown to be free of the sign problem. In these systems, instead of the determinant itself being factorizable, the eigenvalues of the corresponding matrix are complex-conjugate paired, and real eigenvalues are doubly degenerate; thus, the determinant is non-negative valued. Recently, the Majorana HS decomposition was introduced in QMC simulations [27,28]. It is applied to spinless fermion models with repulsive interactions at the particle-hole symmetric point. For some of the above mentioned models, the positivity of fermion determinants can be understood from the algebraic structure of the orthogonal split group $O(N,N)$ [29,30].

The sign structures of the ground state wave functions of quantum lattice models are closely related to the reflection positivity of the Hamiltonian. The concept of reflection positivity was first introduced in the context of quantum field theory [31]. Its main application in condensed matter physics started from Lieb's work on the spin reflection positivity in the Hubbard model [32,33], and was recently applied to systems with Majorana reflection positivity [34–36]. For interacting fermion systems with these reflection positivities, it can be shown that their ground state wave functions are non-negative under certain suitably defined bases. However, these basis states are often nonlocal in real space, which is inconvenient for use in QMC simulations.

In this Letter, we explore the QMC sign problem of lattice fermions from the perspective of Majorana reflection positivity and Majorana Kramers positivity defined below. We use the Majorana fermion representation, because it allows any fermionic systems, whether fermion number conserving or not, to be treated on an equal footing. In the framework of the determinantal QMC algorithm, the statistical weight in the sampling is replaced by the trace of exponentials of fermion bilinears resulting from the HS decomposition, which is evaluated as a determinant. A HS decomposition is said to be a "positive decomposition" if all the generated determinants are positive semidefinite. Below, we show that there are at least two kinds of positive decompositions that lead to QMC simulations free of the sign problem. We dub them Majorana reflection positive decomposition and Majorana Kramers positive decomposition, respectively. These do not exhaust all positive decompositions. They do, however, cover nearly all the interacting lattice fermion models that are previously known to be sign-problem free. From these decompositions, we also identify a number of new models that are free of the sign problem.

Let us begin with the determinantal QMC algorithm for a general lattice model of Dirac fermions. The Hamiltonian H is a sum of a quadratic kinetic energy term H_0 and an interaction term of four-fermion operators H_I [1,2,37]. After the HS decomposition, the partition function Z is expressed as

$$Z = \mathrm{Tr} e^{-\beta H} = \lim_{M\to\infty} \sum_p \rho_p, \tag{1}$$

$$\rho_p = \mathrm{Tr} \prod_{k=1}^{M} e^{-\tau H_0} e^{-\tau H_I(\eta_k)}, \tag{2}$$

where β is the inverse temperature, $\tau = \beta/M$ is the discrete time interval, and $p = \{\eta_M(\{i\}), \ldots \eta_k(\{i\}), \ldots, \eta_1(\{i\}), i = 1, \ldots, N\}$ represents a time sequence of the HS-field distributions with N the lattice size. The decoupled interaction $H_I(\eta_k)$ contains only two-fermion terms, and depends on the time-step size τ and the spatial distribution of the HS fields $\eta_k(\{i\})$. The value of ρ_p can be determined by tracing out the fermion degrees of freedom in H_0 and H_I. The formula for determining ρ_p is given in the Supplemental Material, Sec. I [38].

At each lattice site, a Dirac fermion can be represented using two Majorana fermions. Thus, the original N Dirac fermions can be expressed in terms of $2N$ Majorana fermions. We divide these $2N$ Majorana fermions into two groups, $\gamma_i^{(1)}$ and $\gamma_i^{(2)}$ $(1 \le i \le N)$, and define their Clifford algebra operators as [36]

$$\Gamma_\alpha^+ = i^{[m/2]} \gamma_{i_1}^{(1)} \ldots \gamma_{i_m}^{(1)}, \qquad \Gamma_\alpha^- = (-i)^{[m/2]} \gamma_{i_1}^{(2)} \ldots \gamma_{i_m}^{(2)}, \tag{3}$$

where α represents a sequence $\{i_1, i_2, \ldots, i_m\}$ with $1 \le i_1 < \cdots < i_m \le N$, and $[x]$ equals the largest integer less than or equal to x. $\Gamma_\alpha^\pm$ is said to be even (odd) if m is even (odd). The reflection operation θ is defined as an antilinear automorphism map: $\theta(i) = -i$, $\theta(\gamma_i^{(1)}) = \gamma_i^{(2)}$, and $\theta(\gamma_i^{(2)}) = \gamma_i^{(1)}$. Clearly, $\theta^2 = 1$ and $\theta(\Gamma_\alpha^\pm) = \Gamma_\alpha^\mp$. A bosonic operator O is Majorana reflection symmetric if $\theta(O) = O$, and is Majorana reflection positive if it further satisfies the condition [34,35]

$$\mathrm{Tr}[Q \circ \theta(Q) O] \ge 0, \tag{4}$$

where $Q = \sum_\alpha c_\alpha \Gamma_\alpha^+$ is an arbitrary operator in the algebra spanned by the Γ^+ matrices with the c_α's the complex coefficients, and $Q \circ \theta(Q) = \sum_{\alpha\beta} c_\alpha c_\beta^* \Gamma_\alpha^+ \Gamma_\beta^-$.

In the Majorana representation, the bilinear terms in the expression of ρ_p, including H_0 and $H_I(\tau_k)$, each can be expressed as

$$H_{\mathrm{bl}} = \gamma^T V \gamma, \tag{5}$$

where $\gamma^T = (\gamma_i^{(1)}, \gamma_i^{(2)})^T$ and V is a $2N \times 2N$ antisymmetric matrix. V is the coefficient matrix of H_0 or $H_I(\tau_k)$ in the Majorana representation.

Majorana reflection positive decomposition.—V is defined as a Majorana reflection positive kernel if it can be represented as

$$V = \begin{pmatrix} A & iB \\ -iB^T & A^* \end{pmatrix}, \tag{6}$$

where A and B are $N \times N$ matrices. A is complex antisymmetric satisfying $A^T = -A$. $B = B^\dagger$ is a Hermitian matrix, which is either positive semidefinite or negative semidefinite. (B can be either positive or negative semidefinite because, after a gauge transformation $\gamma_j^{(2)} \to -\gamma_j^{(2)}$, B becomes $-B$ and A remains unchanged.) A HS decomposition satisfying this condition will be called a Majorana reflection positive decomposition.

Theorem 1: ρ_p is positive semidefinite if all the coefficient matrices of the bilinear fermion terms in Eq. (2) are Majorana reflection positive kernels.
This theorem can be proved in two steps. The first is to show that if V is a Majorana reflection positive kernel, then $\exp(-\tau\gamma^T V \gamma)$ is reflection positive. A proof on this was actually already given in Ref. [35]. This means that ρ_p is just the trace of a product of a series of reflection positive operators determined by the exponentials of the bilinear fermion operators H_0 and $H_I(\eta_k)$ in Eq. (2). The second step is to show that the product of a series of reflection positive operators is also reflection positive and its trace is non-negative. A proof of this, as a lemma, is given in the Supplemental Material, Sec. II [38]. Combining the above results, we have $\rho_p \ge 0$. Thus, the system is sign-problem free in QMC simulations if all the kernels in Eq. (2) are Majorana reflection positive. The Majorana reflection can be regarded as a generalization of the PT transformation discussed in Refs. [39,40]. However, this symmetry alone does not leads to the positivity of ρ_p. For example, if B is

not positive semidefinite, $\exp(-\tau\gamma^T V\gamma)$ remains Majorana reflection symmetric, but is no longer Majorana reflection positive. In this case, ρ_p is not always positive definite.

Despite its seeming simplicity, Theorem 1 covers all two- and higher-dimensional interacting fermion models previously known to be sign-problem free in determinantal QMC simulations, without imposing explicitly the TR invariance in the HS decomposition. These include the Hubbard model and its variations [2,18,19], the interacting spinless fermion model [27,28], and other models whose coefficient matrices in the Dirac fermion representation have the orthogonal split $O(N,N)$ group algebra structure [29]. Below, we discuss two such examples, one for spinless fermions and the other for spin-1/2 systems, and prove they are sign-problem free in new parameter regions unknown before.

The first example is an interacting spinless fermion model defined on a bipartite lattice. The model Hamiltonian is

$$H_0 = -\sum_{i,j\in A} c_i^\dagger B_{1,ij} c_j + \sum_{i,j\in B} c_i^\dagger B_{2,ij} c_j + \sum_{i\in A, j\in B} (c_i^\dagger F_{ij} c_j + \text{H.c.}), \tag{7}$$

$$H_I = \sum_{ij} V_{ij}\left(n_i - \frac{1}{2}\right)\left(n_j - \frac{1}{2}\right), \tag{8}$$

where $n_i = c_i^\dagger c_i$. B_1 and B_2 are real symmetric matrices, both of which are positive semidefinite (or, equivalently, negative semidefinite). F is an arbitrary real matrix. $V_{ij} \ge 0$ if i and j belong to different sublattices, and $V_{ij} \le 0$ otherwise.

H_I can be decomposed into a bilinear form by taking the following HS transformation:

$$e^{-\tau V_{ij}(n_i-\frac{1}{2})(n_j-\frac{1}{2})} = \frac{1}{2} e^{-(\tau V_{ij}/4)} \sum_{\eta=\pm} e^{\eta\lambda_{ij}(c_i^\dagger c_j + \nu c_j^\dagger c_i)}, \tag{9}$$

where $\nu = -1$ if i and j belong to the same sublattices and $\nu = +1$ otherwise. In Eq. (9), η is a discrete local HS field, and λ_{ij} is determined by the equation $\sqrt{\nu}\lambda_{ij} = \cosh^{-1}\exp(\tau V_{ij}/2)$.

It is simple to verify that both H_0 and the decoupled interaction terms in the exponent of Eq. (9) can be cast into the form

$$H'_{\text{bl}} = \sum_{i,j\in A} c_i^\dagger (C_{ij} - B_{1,ij}) c_j + \sum_{i,j\in B} c_i^\dagger (D_{ij} + B_{2,ij}) c_j + \sum_{i\in A, j\in B} (c_i^\dagger F_{ij} c_j + \text{H.c.}), \tag{10}$$

where C and D are real antisymmetric matrices satisfying $C = -C^T$ and $D^T = -D$. In the Supplemental Material, Sec. III. A [38], it is shown that the matrix kernel of H'_{bl} is Majorana reflection positive. Therefore, the interacting spinless model $H_0 + H_I$ is sign-problem free, according to Theorem 1.

If both B_1 and B_2 vanish, the above interacting fermion Hamiltonian defined on the honeycomb lattice is the model studied in Refs. [27–29]. It can be extended to include the on-site staggered chemical potential term, and remains sign-problem free [29,41]. This is equivalent to only keeping the diagonal terms of $B_{1,2}$. Generally speaking, in the presence of $B_{1,2}$, Eqs. (7) and (8) do not possess the particle-hole symmetry. For example, consider the case with $B_{1,ij} = \mu\delta_{ij}$ if $i \in A$ and $j \in A$, and $B_{2,ij} = 0$, which is equivalent to applying a uniform chemical potential $\mu/2$ and a staggered on-site potential $(-)^i\mu/2$ to the system. In the weak coupling limit, the single-particle spectrum splits into two bands and the band gap is approximately equal to $\mu/2$, which means that the chemical potential is located right at the bottom of the upper band. At zero temperature, the fermion density remains at half filling. However, with increasing temperature, the fermion density begins to deviate from half filling and the upper band is populated by fermions within an energy window of T starting from the bottom of that band. This implies that a spinless fermion model with repulsive interactions can be simulated without the sign problem away from half filling.

Now let us consider a second example, a spin-1/2 fermion model with Coulomb repulsion, spin-orbit coupling, and spin-flip terms, again defined on a bipartite lattice. This is a generalized Kane-Mele-Hubbard model. The Hamiltonian $H = H_0 + H_I$ is defined by

$$H_0 = -t\sum_{\langle ij\rangle\sigma} c_{i\sigma}^\dagger c_{j\sigma} + i\lambda \sum_{\langle\langle ij\rangle\rangle\sigma} \sigma c_{i\sigma}^\dagger c_{j\sigma} + \sum_{ij} (-)^j h_{ij} c_{i\uparrow}^\dagger c_{j\downarrow} + \text{H.c.}, \tag{11}$$

$$H_I = U\sum_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right), \tag{12}$$

where $c_{i\sigma}$ ($\sigma = \uparrow, \downarrow$) is the annihilation operator of the fermion with spin $\sigma.h_{ij}$ is a real symmetric positive (or, negative) semidefinite matrix. If we only keep the diagonal terms of h_{ij}, they reduce to an in-plane staggered magnetic field distribution. In the limit $\lambda = 0$ and $h_{ij} = 0$, this Hamiltonian becomes the half-filled Hubbard model. For finite λ and h_{ij}, it breaks the SU(2) invariance. In the absence of h_{ij}, the z component of total spin S_z remains conserved. In this case, Eq. (12) is known to be sign-problem free [18,19]. However, in the presence of h_{ij}, both the S_z conservation and the TR symmetry are broken. The previous proof for the absence of the sign problem is no longer valid [18,19].

To show the above model is sign-problem free, let us first consider the following bilinear Hamiltonian of spin-1/2 fermions,

$$H''_{\rm bl} = \sum_{ij} (c^\dagger_{i\uparrow} M_{ij} c_{j\uparrow} + c^\dagger_{i\downarrow} M^*_{ij} c_{j\downarrow}) - \sum_{ij} h_{ij} (c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} + c_{j\downarrow} c_{i\uparrow}), \quad (13)$$

where M_{ij} is an arbitrary $N \times N$ complex matrix. It can be shown that $H''_{\rm bl}$ is Majorana reflection positive. A proof of this is given in the Supplemental Material, Sec. III. B [38].

The Coulomb interaction H_I can be decomposed into a bilinear form by the following HS transformation

$$e^{-\tau U (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})} = \frac{1}{2} e^{\frac{1}{4}\tau U} \sum_{\eta=\pm} e^{i\lambda' \eta (n_{i\uparrow} + n_{i\downarrow} - 1)}, \quad (14)$$

where $\lambda' = \cos^{-1} \exp(-\tau U/2)$. By taking a particle-hole transformation for the down-spin fermion operators $c^\dagger_{j\downarrow} \to (-)^j c_{j\downarrow}$ and keeping the up-spin fermion operators unchanged, the bilinear exponent on the right-hand side of Eq. (14) becomes $i\lambda' \eta (n_{i\uparrow} - n_{i\downarrow})$. Under the same transformation, the t and λ terms in H_0 defined by Eq. (11) remain unchanged, but the h term becomes the second term of Eq. (13). Thus, H_0 is also Majorana reflection positive, and the Kane-Mele-Hubbard model defined in Eq. (12) is free of the QMC sign problem according to Theorem 1.

The absence of the sign problem of the Hamiltonian defined by Eqs. (11) and (12) is actually beyond the framework of Kramers TR-invariant decompositions in the Dirac fermion representation [20,21]. It provides an opportunity to study the effect of TR-symmetry breaking in two-dimensional interacting topological insulators through QMC simulations [42,43]. The h terms, which flip electron spins, can arise from the scattering of magnetic impurities. The magnetic impurities on the edges of a two-dimensional topological insulator can destabilize the helical edge states by opening gaps. The interplay among interaction effects, band structure topology, and magnetic impurities is an interesting topic that deserves further investigation.

Majorana Kramers positive decomposition.—We next present a second theorem for the absence of the sign problem based on the Kramers symmetry structure of Majorana fermions.

Theorem 2: ρ_p is non-negative if there exist two transformation operators S and P such that

$$S^T V S = V^*, \quad (15)$$

$$P V P^{-1} = V, \quad (16)$$

where S is a real antisymmetric matrix satisfying $S^2 = -I$ and $S^T = -S$, P is a symmetric or antisymmetric Hermitian matrix satisfying $P^2 = I$, and P anticommutes with S, i.e., $PS = -SP$.

A proof of this theorem is given in the Supplemental Material, Sec. IV [38]. The HS decomposition satisfying Eqs. (15) and (16) is termed Majorana Kramers positive decomposition. It is a generalization of the Kramers TR-invariant decomposition used in the determinant QMC simulations of Dirac fermions in Refs. [20,21]. Here, S, combined with the complex conjugation C, defines an antiunitary Kramers transformation operator $T = SC$ satisfying $T^2 = -1$. A kernel V that satisfies Eqs. (15) and (16) is also invariant under the antilinear transformation $T' = PSC$. If P is antisymmetric, then T' is also a Kramers operator, satisfying $(T')^2 = -1$, and V is not Majorana reflection symmetric. On the other hand, if P is symmetric, then $(T')^2 = 1$. In this case, V is both Majorana reflection and Kramers symmetric.

Equation (15) ensures that the Majorana coefficient matrix V is symmetric under the TR transformation. But the symmetry alone does not ensure ρ_p to be non-negative. This is because the eigenvalues of $\prod_k \exp(-\tau V_k)$ always appear in pairs: if Λ_α is an eigenvalue, so is Λ_α^{-1}. Moreover, from Eq. (15), it can be shown that Λ^*_α and $(\Lambda^*_\alpha)^{-1}$ are also eigenvalues. If Λ_α is modulus 1, then $\Lambda^*_\alpha = \Lambda^{-1}_\alpha$. In this case, these four eigenvalues reduce to two if Λ_α is not doubly degenerate. According to the expression of ρ_p in terms of the Λ_α's in the Supplemental Material, Sec. I [38], ρ_p may not be positive definite. The condition defined by Eq. (16) adds an extra constraint to the Majorana coefficient matrix V. It enforces the double degeneracy of the eigenvalues of $\prod_k \exp(-\tau V_k)$ when they are modulus 1. This Kramers degeneracy assures $\rho_p \geq 0$.

Theorem 2 is valid independent of the specific representations of S and P. This implies that there is significant flexibility in choosing the HS decomposition scheme. Below, we consider some simple realizations of S and P operators. Assuming the system contains $N = 2L$ sites, we label the lattice sites by two indices (a, i) with $a = 1, 2$ (a can be also regarded as the index for the orbital degrees of freedom) and $i = 1, \ldots, L$, and the corresponding Majorana fermion operators by $\gamma^{(\mu)}_{a,i}$ with $\mu = 1, 2$ the index of the two Majorana fermions at each site. Operator S can then be taken as $S = i\sigma_2 \otimes \tau_0 \otimes I$, where I is the identity matrix in the sector of i, and σ_α and τ_α denote the identity ($\alpha = 0$) and Pauli ($\alpha = 1, 2, 3$) matrices in the sectors of μ and a, respectively. The role of S is to map $\gamma^{(1)}_{a,i}$ to $\gamma^{(2)}_{a,i}$ and $\gamma^{(2)}_{a,i}$ to $-\gamma^{(1)}_{a,i}$.

P can be either antisymmetric or symmetric. An antisymmetric P can be defined as $\sigma_{1,3} \otimes \tau_2 \otimes I$. S and P thus defined can be applied to the interacting fermion model investigated in Refs. [20,21]. For a symmetric P, there are more choices, including any of the following: $\sigma_1 \otimes \tau_\alpha \otimes I$ and $\sigma_3 \otimes \tau_\alpha \otimes I$ ($\alpha = 0,\ 1,\ 3$). For each of these, there exists a corresponding class of V's satisfying Eqs. (15) and (16). For example, for $P = \sigma_1 \otimes \tau_0 \otimes I$, V can be generally expressed as

$$V = \sum_\alpha (\sigma_0 \otimes \tau_\alpha \otimes A_\alpha + i\sigma_1 \otimes \tau_\alpha \otimes B_\alpha), \quad (17)$$

where A_α and B_α with $\alpha = 0$, 1, and 3 are real antisymmetric matrices, and A_2 and B_2 are imaginary symmetric matrices. The interacting fermion models that can be decomposed into the form of Eq. (17) would represent a new class of models without the QMC sign problem. An example of a sign-problem free Hamiltonian that satisfies Eq. (17) is given in the Supplemental Material, Sec. V [38].

Summary.—We have shown that interacting fermion models are free of the sign problem in determinantal QMC simulations if the bilinear Hamiltonians obtained with the HS decomposition possess the Majorana reflection positivity or the Majorana Kramers positivity. The two theorems we have proven cover all the sign-problem-free interacting lattice models that are previously known. They also allow us to identify a number of new interacting fermion models without the QMC sign problem.

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