Solving fermion sign problem in quantum Monte Carlo by Majorana representation

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In this paper, we discover a new quantum Monte Carlo (QMC) method to solve the fermion sign problem in interacting fermion models by employing Majorana representation of complex fermions. We call it “Majorana QMC” (MQMC). Especially, MQMC is fermion sign free in simulating a class of spinless fermion models on bipartite lattices with arbitrary range of interactions. To the best of our knowledge, MQMC is the first auxiliary field QMC method to solve fermion sign problem in spinless (more generally, odd number of species) fermion models. MQMC simulations can be performed efficiently both at finite and zero temperatures. We believe that MQMC has potential of paving a new avenue to solve fermion sign problem in more generic fermionic models.

Introduction: Interacting fermionic quantum systems with strong correlations and/or topological properties have attracted increasing attentions. Universality classes of quantum states of matter in low energy and long distance may be described by field theoretical methods\cite{1,2}. However, in two and higher spatial dimensions, strongly interacting quantum systems are generically beyond the reach of analytical methods in the sense of solving those quantum models in an unbiased way. As an intrinsically-unbiased numerical method, quantum Monte Carlo simulation plays a key role in understanding physics of strongly correlated many-body systems\cite{3–7}. However, in simulating fermionic many-body systems, QMC often encounters the notorious fermion minus-sign problem\cite{8,9}, which arises as a consequence of Fermi statistics\cite{10}. When the sign problem is present, Boltzmann weights in QMC simulations can be negative or even complex such that they cannot be regarded as usual probabilities encountered in simulating classical problems. As a result, relative statistical errors in those QMC simulations scale exponentially with both system sizes and inverse temperature, making it generally unfeasible to accurately simulate such systems with large size and at low temperature\cite{9}. Undoubtedly, generic solutions of fermion sign problems would lead to a great leap forward in understanding correlated electronic systems\cite{9}.

Many QMC algorithms are based on converting an interacting fermion problem into a problem of free fermions interacting with background auxiliary classical fields; the Boltzmann weight depends on determinants of free fermion matrix which is a function of auxiliary fields. In such determinant QMC (DQMC), the determinants can be positive, negative, or even complex. When the determinants are rendered to be positive definite, we say a solution to the fermion sign problem in QMC is found. Conventional strategy of solving fermion sign problem is to find a symmetric treatment of both spin components of electrons such that the Boltzmann weight can be written as the product of two real determinants with the same sign and is then positive definite\cite{11}. For instance, this technique can solve the fermion sign problem in negative \(U\) Hubbard models at any filling as well as the positive \(U\) Hubbard model on bipartite lattices at half-filling because the Boltzmann weight is a product of two identical real determinants of spin-up and spin-down electrons, respectively. When two species of fermions are mixed, the presence of an antiunitary symmetry \(\Theta\) with \(\Theta^2 = -1\) in the fermion matrix may help prove the absence of sign problems\cite{12,10}. It is clear that fermion sign problems in spinless or spin-polarized systems are usually much more difficult to solve because the Boltzmann weight contains only a single determinant and the usual strategy used in even species of fermions cannot be directly applied here.

In this paper, based on Majorana representation of fermions, we propose a genuinely new auxiliary field QMC approach to solve fermion sign problem in spinless fermion models. We observe that each complex fermion can be represented as two Majorana fermions. Consequently, we can express spinless fermion Hamiltonians in Majorana representation and then perform Hubbard-Stratonovich (HS) transformations to decouple interactions by introducing background auxiliary fields. Under certain conditions such as particle-hole symmetry, we can find a symmetric treatment of two species of Majorana fermions, namely the free Majorana fermion Hamiltonian obtained after HS transformations is a sum of two symmetric parts each involving only one species of Majorana fermions, such that the Boltzmann weight is a product of two identical real quantities and is then positive definite. This is the basic idea of the Majorana approach to solve fermion sign problem in spinless or spin-polarized fermion models which we call “Majorana QMC” (MQMC). Note that the MQMC approach proposed here is qualitatively different from the meron-cluster method\cite{17,18} and fermion bags method\cite{19,20} developed previously, all of which are based on continuum-time QMC\cite{20,22}. As far as we know, MQMC is the first QMC approach based on auxiliary fields to solve fermion sign problem in a class of spinless (more generally, odd number of species) fermion models. Moreover, MQMC has an important advantage: it is much more efficient than continuous-time QMC in simulating models at low and zero temperatures; the computation-time cost in MQMC scales as \(\beta \equiv 1/T\) while it scales as \(\beta^3\) in continuous-time QMC\cite{20}.
Majorana quantum Monte Carlo: To explicitly illustrate how MQMC could solve the fermion sign problem in a class of spinless fermion models, we consider the following general Hamiltonian of spinless fermions:

\[ H = H_0 + H_{\text{int}}, \]
\[ H_0 = -\sum_{ij} t_{ij} c_i^\dagger c_j + \text{h.c.}, \]
\[ H_{\text{int}} = \sum_{ij} V_{ij} (n_i - 1/2)(n_j - 1/2), \]

where \( c_i^\dagger \) creates a fermion on site \( i \), \( t_{ij} \) represents hopping integral and \( V_{ij} \) labels density interaction. As we shall show below, the MQMC is fermion-sign-free when the Hamiltonian in Eq. (1) satisfies the following two conditions: (1) \( t_{ij} \neq 0 \) only when \( i, j \) belong to different sublattices; (2) \( V_{ij} > 0 \) when \( i, j \) belong to different sublattices and \( V_{ij} < 0 \) when \( i, j \) belong to same sublattices. With the first condition, it is clear that the model is invariant under particle-hole transformations: \( c_i \rightarrow (-1)^i c_i^\dagger \), where \((-1)^i\) has opposite signs for different sublattices and then describes fermions at half-filling. For simplify, we hereafter consider the model with only nearest-neighbor (NN) hopping \( t \), NN repulsive interaction \( V_1 \), and next-nearest-neighbor (NNN) attractive interaction \( V_2 \) which we call the \( t-V_1-V_2 \) model. The lattice in question can be any bipartite lattice such as honeycomb and square lattices in 2D as well as cubic and diamond lattices in 3D. Generalizing the MQMC method to models with longer-range hopping/interactions will be straightforward. It is interesting to note that the \( t-V_1-V_2 \) spinless fermion model on the honeycomb lattice feature very interesting phases including quantum anomalous Hall (QAH) phases\(^{24}\) and pair density wave (PDW) phases\(^{25}\). Moreover, it has been shown from RG analysis that space-time supersymmetry (SUSY) emerges at the critical points between the Dirac semimetal and PDW phases\(^{25}\). From the mean-field phase diagram of the \( t-V_1-V_2 \) model shown in Fig. 1, MQMC is fermion sign free in the phase region including both Dirac semimetal and charge density wave (CDW) phases\(^{22}\).

In statistical physics, a key quantity is the partition function. QMC methods are designed to simulate partition functions in a statistical fashion. For the \( t-V_1-V_2 \) model, the partition function after Trotter decomposition is given by

\[ Z = \text{Tr} \left[ e^{-\beta H} \right] \approx \text{Tr} \left[ \prod_{n=1}^{N_\tau} e^{-\beta H_0(n) \Delta \tau} e^{-\beta H_{\text{int}}(n) \Delta \tau} \right], \]

where \( \Delta \tau N_\tau = \beta \) and the approximation is good for small \( \Delta \tau \) or large \( N_\tau \). HS transformations can be applied to decouple fermion interactions into non-interacting terms interacting with background auxiliary fields. Usual HS decoupling in density channels normally result in minus sign problem in QMC because the Boltzmann weight is a single determinant. However, we observe that the Hamiltonian can be rewritten in terms of Majorana fermions and there are two species of Majorana fermions. In Majorana representation, complex fermions operators are given by:

\[ c_i = \frac{1}{2} (\gamma_i^1 + i \gamma_i^2), \quad c_i^\dagger = \frac{1}{2} (\gamma_i^1 - i \gamma_i^2), \]

which enable us to rewrite the Hamiltonian as follows:

\[ H_0 = \frac{it}{2} \sum_{\langle ij \rangle} (\gamma_i^1 \gamma_j^1 - \gamma_i^2 \gamma_j^2), \]
\[ H_{\text{int}} = -\frac{V_1}{4} \sum_{\langle ij \rangle} (\gamma_i^1 \gamma_j^1)(\gamma_i^2 \gamma_j^2) - \frac{V_2}{4} \sum_{\langle\langle ij \rangle\rangle} (\gamma_i^1 \gamma_j^1)(\gamma_i^2 \gamma_j^2), \]

where gauge transformations \( c_i \rightarrow ic_i \) for \( i \) in only one sublattice were implicitly made so that \( H_0 \) can be written symmetrically in the two components of Majorana fermions. Now, it is clear that we should perform HS transformations in Majorana hopping channels instead of density channels as done in usual QMC methods. Explicitly, HS transformations for interactions in \( H_{\text{int}} \) in MQMC are given by

\[ e^{-\frac{\lambda_1}{2} (i \gamma_i^1 \gamma_j^1)(i \gamma_i^2 \gamma_j^2)} = \sum_{\sigma_{ij} = \pm 1} \frac{1}{2} \lambda_1 \sigma_{ij} (i \gamma_i^1 \gamma_j^1 + i \gamma_i^2 \gamma_j^2) e^{-\frac{\lambda_1}{2} \Delta \sigma}, \]
\[ e^{-\frac{\lambda_2}{2} (i \gamma_i^1 \gamma_j^1)(i \gamma_i^2 \gamma_j^2)} = \sum_{\sigma_{ij} = \pm 1} \frac{1}{2} \lambda_2 \sigma_{ij} (i \gamma_i^1 \gamma_j^1 - i \gamma_i^2 \gamma_j^2) e^{\frac{\lambda_2}{2} \Delta \sigma}, \]

where \( \lambda_1 \) and \( \lambda_2 \) are constants determined through \( \cosh(2\lambda_1) = e^{-\frac{\lambda_1}{2} \Delta \sigma} \) and \( \cosh(2\lambda_2) = e^{-\frac{\lambda_2}{2} \Delta \sigma} \), respectively. Note that in Eq. (7) the signs of \( \gamma^1 \) hopping terms are opposite to \( \gamma^2 \) hopping terms in the HS decompositions of NNN interaction because \( V_2 < 0 \). The same signs are

FIG. 1. The quantum phase diagram of the \( t-V_1-V_2 \) spinless fermion model on the honeycomb lattice as a function of \( V_1 \) and \( V_2 \). Here “QAH” and “CDW” label quantum anomalous Hall and sublattice-CDW, respectively; “PS” represents phase separation; PDW labels pair density wave (or FFLO phases). At the PDW criticality the \( N = 2 \) space-time SUSY emerges in low energy and long distance\(^{25}\). The shaded region is fermion sign free in MQMC simulations.
obtained for decoupling of NN interactions in Eq. (6) because \( V_1 > 0 \). It is now clear that the free fermion Hamiltonian after the HS transformations is a sum of two parts each of which involves only one component of Majorana fermions. This makes sign problem free possible in the MQMC simulations because the Boltzmann weight can be positive definite, which we shall show below.

Note that auxiliary fields \( \sigma_{ij}(n) \) should be introduced independently for each discrete imaginary time \( n \). As a result, the partition function is a sum over Boltzmann weight which is a function of auxiliary field configurations in space-time, as given by

\[
Z = \sum_{\{\sigma\}} W(\{\sigma\}),
\]

where \( n = 1, \cdots, N_r \) labels the discrete imaginary time and up to an unimportant constant the Boltzmann weight \( W(\{\sigma\}) \) is given by

\[
W(\{\sigma\}) = \text{Tr} \left[ \prod_{n=1}^{N_r} e^{\sum_{a=1}^2 \frac{i}{2} \tilde{\gamma}^a h^a(n) \gamma^a} \right],
\]

where \( \tilde{\gamma}^a \) represents the transpose of \( \gamma^a \) and \( h^a(n) \) is a \( N \times N \) matrix (\( N = \) the number of lattice sites) is given by

\[
h^a_{ij}(n) = i \left[ \frac{t}{2} \Delta \delta_{ij} + \lambda_1 \sigma_{ij}(n) \delta_{ij} \pm \lambda_2 \sigma_{ij}(n) \delta_{ij} \right],
\]

where \( \delta_{ij} = 1 \) if \( ij \) are NN sites and 0 otherwise; similarly \( \delta_{ij} = 1 \) only if \( ij \) are NNN sites. Now, we can trace out the Majorana fermions since they are free, as shown in Supplemental Material. Because the two components of Majorana fermions are decoupled, tracing out Majorana fermions can be done independently and the Boltzmann weight is a product of two factors

\[
W(\{\sigma\}) = W_1(\{\sigma\})W_2(\{\sigma\}),
\]

where

\[
W_a(\{\sigma\}) = \left\{ \det \left[ \prod_{n=1}^{N_r} e^{h^a(n)} + \prod_{n=N_r+1}^{2N_r} e^{-h^a(n)} \right] \right\}^{\frac{1}{2}}.
\]

Note that there is sign ambiguity when taking a square root, similar to the case of Pfaffian as a square root of determinants.

**Fermion sign-problem free:** Now we show that the Boltzmann weight is always positive definite by proving that \( P_1(\{\sigma\}) = P_2(\{\sigma\}) \). A key observation is that the Hamiltonian \( \tilde{h}^1(n) \equiv \tilde{\gamma}^1 h^1(n) \gamma^1 \) of Majorana fermions \( \gamma^1 \) can be mapped to a Hamiltonian identical to \( \tilde{h}^2(n) \equiv \tilde{\gamma}^2 h^2(n) \gamma^2 \) by the following time-reversal transformation and gauge transformation:

\[
T : \gamma^1_i \rightarrow \gamma^1_i, \quad \tilde{T} : \gamma^1_i \rightarrow (-1)^i \gamma^1_i.
\]

Namely, \( \tilde{\gamma}^1 h^1(n) \gamma^1 \rightarrow \tilde{\gamma}^1 h^2(n) \gamma^1 \) under \( TG \). Because the gauge transformation above does not change the results of tracing out Majorana fermions and the time-reversal transformation complex conjugates the results of tracing out Majorana fermions, we obtain

\[
W_1(\{\sigma\}) = W_2(\{\sigma\}),
\]

which renders the Boltzmann weight \( W(\{\sigma\}) = W_1(\{\sigma\})W_2(\{\sigma\}) \geq 0 \) for any auxiliary field configuration \( \{\sigma\} \). Explicitly, it is

\[
W(\{\sigma\}) = \text{det} \left[ \prod_{n=1}^{N_r} e^{h^a(n)} + \prod_{n=N_r+1}^{2N_r} e^{-h^a(n)} \right],
\]

where \( a = 1 \) or 2, which gives rise to the same result. This proves that the MQMC algorithm can solve fermion sign problem in such class of models consisting of spinless fermions. It is the central result in this paper.

**Projector MQMC:** The MQMC algorithm above simulates finite-temperature partition function in the grand canonical ensemble by computing the trace shown in Eq. (9). If one is interested in ground state properties, it is of advantage to use the projector algorithm to carry out QMC since projector QMC is often more efficient than finite-temperature QMC. The expectation value of an operator \( O \) in the ground state is given by

\[
\langle \psi_0 | O | \psi_0 \rangle = \lim_{\theta \rightarrow \infty} \frac{\langle \psi_T | e^{-\theta H} O e^{-\theta H} | \psi_T \rangle}{\langle \psi_T | e^{-2\theta H} | \psi_T \rangle},
\]

where \( | \psi_0 \rangle \) is the ground state and \( | \psi_T \rangle \) is a trial wave function which we assume has a finite overlap with the true ground state. Here, \( Z_T \equiv \langle \psi_T | e^{-2\theta H} | \psi_T \rangle \) plays the role of usual partition functions and need to be expressed as a sum of Boltzmann weights. In practice, a Slater-determinant wave function describing non-interacting fermions is often chosen as the trial wave function in projector QMC:

\[
| \psi_T \rangle = \prod_{a=1}^{N_f} \langle c^\dagger P \rangle_0 | 0 \rangle,
\]

where \( P \) is a \( N \times N_f \) matrix (\( N_f \) labels the number of fermions). Usually, \( | \psi_T \rangle \) is an eigenvector of the non-interacting part of the Hamiltonian in question, namely \( H_0 \) in Eq. (11). In Majorana representation of fermions, \( \gamma^1 \) and \( \gamma^2 \) Majorana fermions are decoupled in \( H_0 \); consequently \( | \psi_T \rangle \equiv | \psi_1 \rangle \otimes | \psi_2 \rangle \). By introducing similar HS transformations and auxiliary fields \( \{\sigma\} \) as above, the “partition function” is obtained as a sum of Boltzmann weight \( W(\{\sigma\}) \) over auxiliary field configurations: \( Z_T = \sum_{\{\sigma\}} W(\{\sigma\}) \). Since \( \gamma^1 \) and \( \gamma^2 \) Majorana fermions are decoupled after the HS transformation, we again obtain \( W(\{\sigma\}) = W_1(\{\sigma\})W_2(\{\sigma\}) \), where

\[
W_a(\{\sigma\}) = \text{det} \left[ \prod_{n=1}^{N_r} e^{\sum_{a=1}^2 \frac{i}{2} \tilde{\gamma}^a h^a(n) \gamma^a} \right] | \psi_T \rangle.
\]
Similarly, \( W_1(\{\sigma\}) = W_2^*(\{\sigma\}) \) because of the symmetry \( TG \). As shown in the Supplemental Material, the Boltzmann weight is given by

\[
W(\{\sigma\}) = \left| \det \left\{ P_a \prod_{n=1}^{N_x} \exp(\alpha(n)) P_a \right\} \right|,
\]

where \( \alpha = 1 \) or 2 and \( P_a \) is the projection matrix constructed from \( |\phi^a_t\rangle \). Consequently, the projector MQMC is also free from fermion sign problem for a class of spinless fermion models.

**Physical observables in MQMC:** One important advantage of DQMC algorithms is that physical observables can be obtained conveniently. For instance, time and space dependent Green’s function can be computed directly in terms of DQMC algorithm. We show below that the computation of physical observables in MQMC is similarly convenient as that in DQMC algorithm.

In QMC, physical observables can be related to single-particle Green’s function: \( G_{ij} = \langle c_i^\dagger c_j \rangle \), where the average is done stochastically over auxiliary field configurations. In Majorana representation, it is given by

\[
\langle c_i^\dagger c_j \rangle = \langle \gamma_i^1 \gamma_j^1 \rangle + \langle \gamma_i^2 \gamma_j^2 \rangle,
\]

where we used the results of \( \langle \gamma_i^1 \gamma_j^1 \rangle = 0 \) which is a consequence of the decoupling of the two species of Majorana fermions after the HS transformation. To obtain the Green’s functions, we only need to compute \( \langle \gamma_i^1 \gamma_j^1 \rangle \) and \( \langle \gamma_i^2 \gamma_j^2 \rangle \). Because the two species of Majorana fermions are related by the symmetry transformation \( TG \), we obtain \( W_1(\{\sigma\}) = W_2^*(\{\sigma\}) \). As shown in Supplementary Material, it is straightforward to evaluate the Majorana Green’s function \( \langle \gamma_i^a \gamma_j^b \rangle \) in MQMC. Employing Wick’s theorem, higher order correlation functions, including density-density correlations and pair-pair correlations, can be obtained in MQMC from single-particle Green’s functions. For instance, the equal-time density-density correlations are

\[
\langle c_i^\dagger c_i^\dagger c_j c_j \rangle = \left[ \langle \gamma_i^1 \gamma_j^1 \rangle + \langle \gamma_i^2 \gamma_j^2 \rangle \right] \left[ \langle \gamma_i^1 \gamma_j^1 \rangle + \langle \gamma_i^2 \gamma_j^2 \rangle \right].
\]

**Entanglement entropy in MQMC:** It is increasingly realized that quantum entanglement could play a key role in understanding quantum many-body systems\[29,32\]. For a pure state or thermal states with density matrix \( \rho \), entanglement entropy between subsystems \( A \) and the rest \( \bar{A} \) is defined as the von Neumann entropy \( S_{A|\bar{A}} = -\text{Tr}[\rho_A \log \rho_A] \) where \( \rho_A = \text{Tr}_{\bar{A}} \rho \) is the reduced density matrix by tracing over the Hilbert space of \( \bar{A} \). It is one of the main physical quantities to characterize quantum entanglement\[33\]. It is still challenging for auxiliary field QMC algorithms to evaluate von Neumann entropy. Nonetheless, it was shown recently that auxiliary-field QMC can provide an efficient way to evaluate Renyi entropy, defined as \( S_n = -\frac{1}{n-1} \log[\text{Tr}(\rho_A^n)] \) by simulating the reduced density matrix \( \rho_A \) expressed in terms of Green’s function\[34,35\]. Specifically, in auxiliary-field QMC algorithms such as DQMC, the reduced density matrix is \( \rho_A = \sum \sigma W(\sigma) \rho_A^\sigma \), where \( \{\sigma\} \) labels auxiliary field configuration with Boltzmann weight \( W(\sigma) \) and

\[
\rho_A = \det[\mathbb{I} - G_{A\sigma} e^{-c \log(G_{A\sigma}^{-1})}],
\]

where \( G_{A\sigma} \equiv \langle c_i^\dagger c_j \rangle_\sigma \) is the Green’s function of region \( A \) evaluated with respect to the free-fermion Hamiltonian with auxiliary field configuration \( \sigma \); \( c \) and \( c^\dagger \) above are also restricted to region \( A \). In MQMC, we can obtain the Green’s function of complex fermions by evaluating correlation functions of Majorana fermions, as is shown in [Eq. (20)]. As a result, Renyi entropy can also be evaluated efficiently in MQMC as long as it is free of fermion sign problem. For example, the Renyi entropy \( S_2 \) is given via \[34\]:

\[
S_2 = -\log \left\{ \sum_{\sigma,\sigma'} W(\sigma)W(\sigma') \left[ \det \left[ G_{A\sigma} G_{A\sigma'} \right] \right] + (1 - G_{A\sigma})(1 - G_{A\sigma'}) \right\}.
\]

**Concluding remarks:** We have shown that MQMC, as a new auxiliary field QMC approach, can solve fermion sign problem in a class of spinless fermion models by utilizing Majorana representation of complex fermions. It will be straightforward to generalize the current MQMC algorithm to solve the fermion sign problem in interacting quantum models with even or odd number of fermion species. Particularly, such MQMC fermion-sign free models include the \( SU(N) \) Hubbard model on bipartite lattices with \( N = \text{odd} \) and negative-\( U \) Hubbard interactions. Because MQMC can efficiently simulate systems with relatively large size and at zero temperature, it can be employed to investigate strong correlated phases as well as universal behaviors at quantum critical points\[36\]. For instance, performing MQMC simulations for the \( t-V_1-V_2 \) honeycomb model in the sign-free region will help to understand better the CDW (or nematic) quantum critical point which is described by a putative Gross-Neveu transition\[22,37\].

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[4] R. Blankenbecler, D. J. scalapino, and R. L. Sugar, Phys. Rev. D 24, 2278 (1981).
Now we show that the trace of exponentials of bilinear Majorana fermion operators can be expressed as the square root of a determinant (nonetheless, it is formally not a Pfaffian as shown below).

First, we evaluate the trace of a single exponential of bilinear Majorana fermion operators. Suppose \( \hat{h} = \sum_{ij} \gamma_i h_{ij} \gamma_j / 2 \) where \( h_{ij} = -h_{ji} \) is purely imaginary and we need to compute \( \text{Tr}[e^{-\Delta \tau h}] \). After diagonalizing \( \hat{h} = \sum_{a=1}^{N/2} \epsilon_a c_a^\dagger c_a - \epsilon_a c_a c_a^\dagger \), where \( \pm \epsilon_a \) are eigenvalues of the \( N \times N \) matrix \( \hat{h} \), it is clear that the trace is given by

\[
\text{Tr}[e^{-\Delta \tau h}] = \prod_{a=1}^{N/2} (e^{\Delta \tau \epsilon_a} + e^{-\Delta \tau \epsilon_a}),
\]

which can be reexpressed as the square root of a determinant:

\[
\text{Tr}[e^{-\Delta \tau h}] = \left( \det (e^{\Delta \tau h} + e^{-\Delta \tau h}) \right)^{1/2}.
\]

Intuitively, the square root originates from the fact that Majorana fermions carry only half of degrees of freedom of corresponding Hamiltonian in terms of complex fermions.

Then we show that the product of exponentials of bilinear Majorana fermion operators can be grouped into a single exponential of a bilinear Majorana fermion form. Suppose \( U = \prod_n e^{\Delta \tau h(n)} \), where \( h(n) = 1/2 \sum_{ij} \gamma_i h_{ij}(n) \gamma_j \), and
we would like to evaluate \( \text{Tr}[U] \). By observing that \( e^{-\Delta \tau \hat{h}(n)} \gamma_i e^{\Delta \tau \hat{h}(n)} = \sum_j \gamma_j [e^{-\Delta \tau \hat{h}(n)}]_{ji} \), we obtain

\[
U \gamma_i U^{-1} = \sum_j \gamma_j \left[ \prod_n e^{-\Delta \tau \hat{h}(n)} \right]_{ji},
\]

\[
= \sum_j \gamma_j \left[ e^{-\Delta \tau \hat{h}'} \right]_{ji},
\]

where a \( N \times N \) matrix \( h' \) is defined. Accordingly, we introduce bilinear Majorana fermion operators: \( \hat{h}' = \frac{1}{2} \sum_{ij} \gamma_i h'_ij \gamma_j \). Now, we can show that the trace of the product of exponentials of the Majorana fermions bilinear operator is given by the square root of a determinant:

\[
\text{Tr} \left[ \prod_n e^{-\Delta \tau \frac{1}{2} \hat{h}(n) \gamma} \right] = \text{Tr} \left[ e^{-\Delta \tau \frac{1}{2} \hat{h}' \gamma} \right],
\]

\[
= \left[ \det \left( e^{\Delta \tau h'} + e^{-\Delta \tau h'} \right) \right]^{\frac{1}{2}},
\]

\[
= \left\{ \det \left[ \prod_n e^{\Delta \tau \hat{h}(n)} + \left( \prod_n e^{\Delta \tau \hat{h}(n)} \right)^{-1} \right] \right\}^{\frac{1}{2}},
\]

which proves the result in Eq. (11).

B: Projector QMC in Majorana representation

We now prove the result in Eq. (19). To compute \( W_a(\{\sigma\}) \), we compute its square first as follows:

\[
W^2_a(\{\sigma\}) = \langle \psi^a_T \mid \prod_{n=1}^{N_f} e^{\frac{1}{2} \gamma^n h^n(n)} \gamma^n \mid \psi^a_T \rangle \langle \phi^a_T \mid \prod_{n=1}^{N_f} e^{\frac{1}{2} \gamma^n h^n(n)} \eta^n \mid \phi^a_T \rangle,
\]

\[
= \langle \psi^a_T \otimes \phi^a_T \mid \prod_{n=1}^{N_f} e^{\frac{1}{2} \gamma^n h^n(n)} \gamma^n + \frac{1}{2} \gamma^n h^n(n) \eta^n \mid \psi^a_T \otimes \phi^a_T \rangle,
\]

where \( \eta^n \) are the “ghost Majorana fermions” which are independent from \( \gamma^n \) but have the same Hamiltonian and ground state wave function as \( \gamma^n \). When combining \( \eta^n \) and \( \gamma^n \) into complex fermions \( d_j \equiv (\gamma_j^0 + i \eta_j^0)/2 \), we obtain

\[
W^2_a(\{\sigma\}) = \langle \psi^a_T \otimes \phi^a_T \mid \prod_{n=1}^{N_f} e^{d_j h^n(n) d} \mid \psi^a_T \otimes \phi^a_T \rangle,
\]

\[
= \det \left\{ \prod_{n=1}^{N_f} e^{h^n(n)} \right\}_{P^a},
\]

where \( P^a \) is a \( N \times N_f \) projector matrix defined through \( \mid \psi^a_T \otimes \phi^a_T \rangle = \prod_n (d^a P^a_n) \mid 0 \rangle \). Because \( W_1(\{\sigma\}) = W^*_2(\{\sigma\}) \), we prove Eq. (19) as follows:

\[
W(\{\sigma\}) = \left| \det \left\{ \prod_{n=1}^{N_f} e^{h^n(n)} \right\}_{P^a} \right|.
\]
Appendix C: Green’s functions of Majorana fermions

We have shown that Green’s functions of original complex fermions can be expressed in terms of Green’s functions of Majorana fermions $G_{ij}^a \equiv \langle \gamma^a_i \gamma^a_j \rangle$ ($a = 1, 2$), which can be evaluated in MQMC as follows:

$$G_{ij}^a = \sum_{\{\sigma\}} W(\{\sigma\}) \langle \gamma^a_i \gamma^a_j \rangle_{\sigma},$$ (S13)

$$= \sum_{\{\sigma\}} W(\{\sigma\}) \frac{\text{Tr} \left[ \gamma^a_i \gamma^a_j \prod_{n=1}^{N_{\tau}} e^{-\tilde{\gamma}^a h^a(n)\gamma^a} \right]}{\text{Tr} \left[ \prod_{n=1}^{N_{\tau}} e^{-\tilde{\gamma}^a h^a(n)\gamma^a} \right]},$$ (S14)

$$= \frac{1}{2} \sum_{\{\sigma\}} W(\{\sigma\}) \left\{ \prod_{n=1}^{N_{\tau}} e^{h^a(n)} - \prod_{n=1}^{N_{\tau}} e^{-h^a(n)} \left[ \prod_{n=1}^{N_{\tau}} e^{h^a(n)} + \prod_{n=1}^{N_{\tau}} e^{-h^a(n)} \right]^{-1} \right\}_{ji},$$ (S15)

where equal-time Green’s functions was implicitly assumed. The factor $1/2$ above comes from the nature of Majorana fermions.