Semigroup Approach to the Sign Problem in Quantum Monte Carlo Simultions

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We propose a new framework based on the concept of semigroup to understand the fermion sign problem. By using properties of contraction semigroups, we obtain new sufficient conditions for quantum lattice fermion models to be sign-problem-free. Many previous results can be considered as special cases of our new results. As a direct application of our new results, we construct a new class of sign-problem-free fermion lattice models, which cannot be understood by previous frameworks. This framework also provides an interesting aspect in understanding related quantum many-body systems. We establish a series of inequalities for the sign-problem-free fermion lattice models satisfy our sufficient conditions.

I. INTRODUCTION

Understanding interacting many-body systems remains a great challenge in current physics research. The quantum Monte Carlo (QMC) method is an important numerical method for this purpose[1–4]. It contains a class of stochastic algorithms based on sampling over different configurations according to some sampling weights derived from the model. However, for many quantum models it is often extremely difficult to express the quantum partition function or expectation values of physical variables in terms of efficiently computable, non-negative real sampling weights. This obstacle, which often hampers the efficiency of QMC simulations seriously, is called the sign problem. It prevents us from getting numerical results for large systems, at low temperature effectively.

Specifically speaking, for auxiliary field quantum Monte Carlo(AFQMC) type algorithms[5, 6] that are frequently used in condensed matter physics, nuclear physics and cold atoms, for each configuration of auxiliary fields the contribution to the partition function can be expressed by the determinant resulting from the fermionic Gaussian integral, which can be computed efficiently. Unfortunately, in general a fermionic Gaussian integral is not necessarily a real number, even less a non-negative real number. For fermion lattice models, the sign problem will lead to an exponential growth of total computational cost as the volume of the system and the inversed temperature get larger[7], if one wants to retain the same numerical accuracy.

Despite the fact that a general unbiased solution to the sign problem is either non-existent or elusive by its very nature[8], a lot of physically interesting models have been shown to be sign-problem-free, which is of great significance to practical numerical studies. For AFQMC and some related methods, a few general frameworks have been proposed to understand sign-problem-free interacting fermion systems. There have been approaches based on the Kramers time-reversal invariance[9–11], the fermion bag[12, 13], the split orthogonal group[14], the Majorana reflection positivity[15], and the Majorana-time-reversal symmetries[16]. Each approach has unified a class of sign-problem-free fermion models and brought new examples of sign-problem-free QMC simulations.

In this work, we propose an essentially new approach to construct fermion models without sign problem. We observe that semigroup structures arise naturally from imaginary-time evolutions, which is made explicit after introducing auxiliary fields. The semigroup is generated by multiplication of exponentials of fermionic quadratic operators. It is not necessarily a group, for the inverse elements of those exponentials may not appear in the calculation. An important particular case is when each element of the semigroup has non-negative trace, the QMC sampling weights are exactly the traces. This fact serves as the stating point of our approach.

A semigroup is a set with element multiplication that satisfies the associative law. Compared with the concept of group, an inverse does not necessarily exist for each element in a semigroup. Semigroups appear frequently in different areas of theoretical research. Every group is also a semigroup. In quantum mechanics, the quantum dynamical semigroup[17] is employed to study the time evolution of open quantum systems, where the concept of semigroup reflects the irreversiblility of time for the concerned physical processes. In quantum field theory and statistical physics, the renormalization group(RG)[18] is actually more like a semigroup than a group, due to the loss of information during RG transformations.

In this work, we are mainly concerned with a special kind of Lie semigroups called the contraction semigroups. We construct two kinds of contraction semigroups. When the parameter region is contained in such semigroups, the fermionic Gaussian integral is always non-negative real. As a result, the related AFQMC calculations do not have any sign problem.

The currently existing approaches mentioned above appear different and unrelated at first glance, but now they can be unified in this new framework. The Kramers time-reversal invariance leads to Kramers pairs of eigenvalues of matrices, which results in the non-negativity of fermion determiants[11]. In Ref. [14], the relation be-

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tween the split orthogonal group and sign-problem-free models has been revealed using some inequality for group elements. Those results have been extended by recent studies[15, 16]. We show that all those approaches based on consideration of symmetries are related to subgroups of the semigroups considered here. We also explain that in the context of the AFQMC sign problem, the condition of Majorana reflection positivity[15] is actually equivalent to one of the two kinds of contraction semigroups treated in this work. In short, to our best knowledge, all the known results for fermion lattice models can be understood in our framework.

Our results open up new possibilities to sign-problem-free Monte Carlo simulations. As an example, we construct a kind of interacting fermion lattice model which involves the paring term, the Kramers time-reversal invariant hopping term, and the interaction term. This class of model is sign-problem-free, which could not find explanation in previous frameworks.

We believe that this framework will find more applications in both numerical and analytical studies. To illustrate the latter case, we establish certain inequalities for the expectation values of physical observables in many-body systems.

II. PROBLEM SETTING

In AFQMC algorithms for interacting fermion lattice models, interaction terms are decoupled by auxiliary fields into fermionic quadratic forms[5, 6, 19]. After integrating out the fermion degrees of freedom, one will obtain an action in terms of auxiliary fields. One can treat this action with random sampling numerically. The sampling weight for each configuration of auxiliary fields usually has the form

$$\begin{aligned} p &= \mathrm{tr}\left(e^{h_1} e^{h_2} \cdots e^{h_k}\right) \\ &= \det\left(I + e^{A_1} e^{A_2} \cdots e^{A_k}\right)^{1/2}. \end{aligned} \tag{1}$$

The expression of sampling weight in Eq. (1) is the main object of study in this work. Here $h_i = \gamma^T A_i \gamma/4$ ($i = 1, \ldots, k$) denote a set of fermionic quadratic forms. They come from both single-body terms and auxiliary field decoupling of interaction terms, and depend on the configuration of auxiliary fields. γ_n ($n = 1, \ldots, 2N$) are Majorana fermion operators, which satisfy anticommutation relations $\{\gamma_l,\, \gamma_m\} = 2\delta_{lm}$. The Majorana fermion basis is used for convenience, it is (unitary) equivalent to the complex fermion basis with N species. Unless we specify a particular example, in principle h_i could contain an arbitrary particle number conserving part and an arbitrary pairing part. That is to say the coefficients $A_i = -A_i^T$ could be arbitrary skew-symmetric complex matrices.

If we do not put any restrictions on h_i, the fermionic Gaussian integral p could be non-positive, due to both the complex nature of the coefficients and the two-valuedness of the spin representation. Under those circumstances statistical sampling methods may fail to obtain desired physical quantities with useful accuracy at reasonable cost. This is the so-called sign problem in AFQMC methods.

In practical calculations, the possible forms of e^{h_i} are given by the quantum partition function. They could come from both the single-body term in the Trotter-Suzuki decomposition and the Hubbard-Stratonovich(HS) transformations for interaction terms. Their inverse elements e^{-h_i}, however, are not necessarily involved in any fermionic Gaussian integrals[20]. By taking products along the imaginary-time axis, they form a semigroup, with elements representing different sorts of paths of the partition function. This observation allows us to study the sign problem in terms of semigroup.

Furthermore, if a Lie semigroup $S \subset Spin\,(2N, \mathbb{C})$ has property $p \geq 0$ for all its elements, then it corresponds to a class of sign-problem-free fermion models. In the following sections, we show that two specific kinds of Lie semigroups indeed possess this good property.

III. DEFINITIONS AND USEFUL FACTS

We list some basic definitions and facts before going into details. For general mathematical accounts of Lie semigroups, the reader may refer to Refs. [21, 22].

For any square complex matrix X, consider an anti-linear symmetry operation $X \mapsto \eta X^\dagger \eta$ given by a Hermitian matrix $\eta = \eta^\dagger$ with $\eta^2 = I$, together with Hermitian conjugation. We say that the matrix is η-Hermitian or η-anti-Hermitian respectively, if it is invariant or changes sign under this transformation. All the square complex matrices X with property $\eta X + X^\dagger \eta \leq 0$ generate a Lie semigroup by taking exponentials and element products. Semigroups of this kind are called contraction semigroups. Equivalently, one can say that the contraction semigroup consists of all the square matrices g that satisfy $g^\dagger \eta g - \eta \leq 0$. They contract the "length" of any vector given by the metric η. Similarly, one can define the expansion semigroup by changing the direction of the inequlity. We will work on the contraction semigroup and leave the expansion case to the reader.

Obviously, the contraction semigroup defined above has the η-unitary group as its maximal subgroup, which is generated by η-anti-Hermitian matrices. Each element g in the contraction semigroup possesses a polar decomposition $g = g_U \exp(X_0)$, where X_0 is η-Hermitian and $\eta X_0 \leq 0$, and g_U belongs to the η-unitary group, i.e., $g_U^\dagger \eta g_U = \eta$. The set of X_0 forms a invariant cone, under adjoint action of the η-unitary group.

Specially, let us consider strict contraction elements, which remain strict contractions when multiplied by any semigroup elements. In strict contraction case $g^\dagger \eta g - \eta < 0$, which implies that $\eta X_0 < 0$ and g cannot have eigenvalues of magnitude 1.

IV. SIGN-PROBLEM-FREE SEMIGROUPS

Let us give the outline of the discussions in this section. Firstly we restrict the range of parameters by an anti-linear symmetry to make the sampling weight p real. Then we observe that p never vanishes for strict contraction elements inside some contraction semigroups, while the non-strict contraction elements can be viewed as some limit of strict contraction elements. These two conditions together ensure that p is non-negative as a continuous function of the coefficients.

Each condition requires a definition of anti-linear involution for complex skew-symmetric matrices. Consider any complex skew-symmetric matrix A. Adopting the Majorana fermion basis, it is natural to assume that those two operations are expressed by real orthogonal transformations acting on A, J_1 and J_2 respectively, along with the complex conjugation.

Firstly, we assume the complex skew-symmetric matrices are fixed under the operation $A \mapsto J_1^T \bar{A} J_1$. Here J_1 could be either symmetric $J_1^2 = I_{2N}$, or skew-symmetric $J_1^2 = -I_{2N}$. It is easy to see that p is real under this assumption.

Secondly, to define a contraction semigroup, J_2 should be chosen to be either symmetric or skew-symmetric, so that J_2 or iJ_2 can serve as the aforementioned indefinite metric η. The coefficient matrices that are not changed under the transformation $A \mapsto J_2^T \bar{A} J_2$ generate the maximal subgroup of the contraction semigroup. Meanwhile, elements in the invariant cone change sign under this operation, $iJ_2 A = -i\bar{A}J_2 \leq 0$. Since A is skew-symmetric, if J_2 were symmetric, the invariant cone would be trivial, i.e., it contains only zero element. Therefore we have to assume J_2 to be skew-symmetric. According to Eq. (1), p is nonzero for any such defined strict contraction element, because the matrix inside the determinant does not have zero eigenvalues.

Finally, we have to check the consistency of the two conditions. The resulting invariant cone should statify both constraints given by J_1 and J_2. However, in order to make our argument stand, we have to ensure that the resulting invariant cone always contains strict contraction elements. This cannot be achieved by an arbitrary choice of J_1 and J_2[23]. Under the current assumption, the only possibility is that J_1 and J_2 satisfy the anticommutation relation $\{J_1,\ J_2\} = 0$. See Supplemental Material[24] for more detailed arguments.

Now we have two sign-problem-free semigroups on which $p \geq 0$, and they are defined by

$$J_1^T A J_1 = \bar{A}, \tag{2}$$

$$i\left(J_2 A - \bar{A} J_2\right) \leq 0. \tag{3}$$

J_1 and J_2 are two anti-commuting, real orthogonal matrices. While J_1 could be symmetric or skew-symmetric, J_2 should be skew-symmetric. If all A_i matrices in Eq. (1) satisfy the conditions above, the corresponding quantum Monte Carlo simulations will be sign-problem-free.

Throughout the above discussions we do not require the Hermitian condition of Majorana fermion operators $\gamma_n = \gamma_n^\dagger$. Instead, the anticommutation relations for Majorana fermion operators are preserved under complex orthogonal transformations of Majorana fermion operators. So the condition for positive trace given above also holds for this complex orthogonal generalization of the Majorana fermion basis.

V. APPLICATIONS

Eq. (2) and Eq. (3) consititute the main result of this work. They cover all the results on sign-problem-free QMC simulations of fermion lattice models known to us.

Firstly, when the inequality in Eq. (3) becomes equality, we will have two anti-linear symmetries $J_1^T A J_1 = J_2^T A J_2 = \bar{A}$. Under this circumstance our result goes back to the known results based on symmetry considerations[15, 16]. In this case parameters actually live in the maximal subgroup of the semigroup. Many models in practical studies fall into this case, which can be simulated by quantum Monte Carlo without sign problem[6, 9–11, 13, 14, 16, 19, 25–33]. Below we list a few important examples.

(a)The negative-U Hubbard models, the positive-U Hubbard models at half-filling on bipartite lattices[26], and the Kane-Mele-Hubbard model[27–29] at half-filling can all be regarded as good examples of this case. For those models J_1 could either be symmetric or skew-symmetric, depending on different choices of the Majorana fermion basis.

(b)A class of interacting spinless fermion models on bipartite lattices at half-filling have been shown to be sign-problem-free using the fermion bag approach[12] for continuous-time quantum Monte Carlo(CTQMC) method[13]. They have also been treated without sign problem using AFQMC under the Majorana fermion basis[32], and using CTQMC under the framework of the split orthogonal group[14]. Actually our result applies to several different kinds of QMC methods despite their differences in practice. That class of spinless fermion models are typical examples of the case with symmetric J_1. Another example is a model for helical topological superconductors with interactions[16].

(c)For the case with skew-symmetric J_1, the related fermion lattice models have Kramers time-reversal invariance [15, 16]. Applications can also be found in high-spin interacting fermion systems, e.g. the nuclear shell model[9] and the high-spin Hubbard model[10, 11]. This sign-problem-free property of Kramers time-reversal invariant models also has applications in the research of high-temperature superconductors[25, 30, 33].

Secondly, when J_1 is symmetric, the parameter region given by Eq. (2) and Eq. (3) coincides with the result obtained from Majorana reflection positivity. To see this clearly, one may choose a Majorana fermion basis such that $J_1 = \sigma_1 \otimes I_N,\ J_2 = i\sigma_2 \otimes I_N$. The fermion degrees of freedom are grouped into two parts under this new basis $\gamma = \begin{pmatrix} \gamma^{(1)} \\ \gamma^{(2)} \end{pmatrix}$, while the condition of reflection symmetry is given by Eq. (2), and the condition of positivity is ensured by Eq. (3). We have $\gamma^T A\gamma = \gamma^{(1)T} B\gamma^{(1)} + \gamma^{(2)T} \bar{B}\gamma^{(2)} + 2i\gamma^{(1)T} C\gamma^{(2)}$, with block matrices B and C. C is positive semidefinite Hermitian matrix. This can be immediately compared to the related definitions in Ref. [15]. All the models studied by the fermion bag approach and the split orthogonal group approach can also be treated by Majorana reflection positivity.

The set of operators with Majorana reflection positivity is closed under multiplication[15, 34], which accounts the semigroup property. Each strict contraction element corresponds to a strictly positive operator in the sense of Majorana reflection positivity. We mention that this strict reflection positivity can also be used to show the uniqueness of the ground state for finite systems[35, 36].

Thirdly, when J_1 is skew-symmetric, the result above implies new sign-problem-free models. For convenience in practical applications, we reexpress our result for this J_1 skew-symmetric case in terms of the complex fermion basis. Without losing generality, we can choose a Majorana fermion basis $\gamma = \begin{pmatrix} \gamma^{(1)} \\ \gamma^{(2)} \\ \gamma^{(3)} \\ \gamma^{(4)} \end{pmatrix}$ so that the two skew-symmetric orthogonal matrices have the form $J_1 = \sigma_x \otimes i\sigma_y \otimes I_{N/2}$, $J_2 = -i\sigma_y \otimes I_2 \otimes I_{N/2}$. Then we define the complex fermion basis as $c_l = \left(\gamma_l^{(1)} + i\gamma_l^{(2)}\right)/2$, $d_l = \left(\gamma_l^{(4)} + i\gamma_l^{(3)}\right)/2$, here $l = 1, \ldots, N/2$ labels different components. There is a one-to-one correspondence between the coefficient matrices A which satisfy the conditions in Eq. (2), and the fermionic quadratic forms with Kramers time-reversal invariance,

$$h = \frac{1}{4}\gamma^T A\gamma = h^{(0)} + h^{(p)}, \tag{4}$$

$$h^{(0)} = \left(c^\dagger,\ d^\dagger\right) M \begin{pmatrix} c \\ d \end{pmatrix} - (c,\ d)\, M^T \begin{pmatrix} c^\dagger \\ d^\dagger \end{pmatrix}, \tag{5}$$

$$h^{(p)} = (c,\ d)\, RK \begin{pmatrix} c \\ d \end{pmatrix} - \left(c^\dagger,\ d^\dagger\right) SK \begin{pmatrix} c^\dagger \\ d^\dagger \end{pmatrix}. \tag{6}$$

M, R, and S are complex coefficient matrices, and $K = i\sigma_y \otimes I_{N/2}$. RK and SK are skew-symmetric, in accordance with the fermion anticommutation relations. The time reversal operation is given by the unitary transformation K followed by a complex conjugation of the coefficients under complex fermion basis. It is not difficult to check that $K^T MK = \bar{M}$, $K^T RK = \bar{R}$, $K^T SK = \bar{S}$. Then the condition in Eq. (3) is now converted to two inequalities for Hermitian matrices R and S, $R \geq 0$, $S \geq 0$ under this complex fermion basis. The particle number conserving part $h^{(0)}$ corresponds to the maximal subgroup of the contraction semigroup, while the pairing term $h^{(p)}$ corresponds to the invariant cone.

Consider a Kramers time-reversal invariant effective band Hamiltonian defined on an arbitrary lattice, with time-reversal symmetry that satisfies $K^2 = -I$. We add an attractive on-site Hubbard-U term to the Hamiltonian. With appropriate HS transformations to decouple the interaction term[37], sign-problem-free AFQMC simulations can be carried out for this type of models[11]. Now we can extend this model by adding a new pairing term, which satisfies the sign-problem-free conditions, to study the proximity effect of superconductivity to topological matters with correlation effects. Actually, by particle-hole transformation one can also map an attractive interaction term to a repulsive one, or a pairing term to a hopping term to study more physical problems in strongly correlated electron systems. Those possibilities have not been shown by any previous research.

We note that for some models both cases, symmetric and skew-symmetric J_1, are suitable, depending on the choice of Majorana basis. Those models correspond to the intersection of the two semigroups. A generalized Kane-Mele-Hubbard model on a bipartite lattice with staggered magnetic field, considered in Ref. [15], can be seen as an example.

For many models the system contains several different kinds of degrees of freedom. Suppose each subsystem satisfies sign-problem-free condition, e.g., with its own choice of matrices J_1 and J_2. If the coupling terms between the two sign-problem-free subsystems are carefully selected, the whole system can still be sign-problem-free. In that case, our sign-problem-free conditions are to be applied to each building block of the whole system. This observation can be useful in the study of multilayer systems.

For sign-problem-free models studied in this work, the partition function can be seen as a summation of contraction semigroup elements. This structure can have interesting consequences, including the sign structure of expectation values of observables. For example, for any positive integer m, we have

$$\mathrm{tr}\left(h_1' g_1 h_2' g_2 \ldots h_m' g_m\right) \geq 0, \tag{7}$$

where the coefficient matrices of fermionic quadratic operators h_s' belong to the invariant cone and g_s can take any elements of the contraction semigroup, $s = 1, \ldots, m$. The proof is straightforward for the case with symmetric J_1 owing to Majorana reflection positivity. Numerical tests suggest that the same property holds when J_1 is skew-symmetric. A rigorous proof is not yet available.

VI. CONCLUSION AND DISCUSSION

In this work we have presented sufficient conditions for sign-problem-free QMC simulations of fermion lattice models. A new framework based on the concept of semigroup has been proposed to understand this problem in a systematic way. New sufficient conditions have been obtained, as stated in Eq. (2) and Eq. (3). All previous results based on symmetry considerations and Majorana reflection positivity can be understood well and unified naturally within our new approach. New sign-problem-free models have been constructed to show the power of our method. Such sign-problem-free interacting fermion models share some general physical properties, as we have demonstrated.

Although we have focused on applications in quantum lattice models in condensed matter physics, our framework is not limited to those cases and can also help with the sign problems in the other branches of physics[38].

We would like to mention that the techniques used in this work can be extended to systems with bosonic degrees of freedom.

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SUPPLEMENTAL MATERIAL

Appendix A: Proof of the skew-symmetry property of J_2

If J_2 were symmetric, for any element A in the invariant cone with metric J_2, let $A' = \left(A + \bar{A}\right)/2$. From $J_2^T A J_2 = -\bar{A}$ we know that $\{J_2,\ A'\} = 0$. Then we would have

$$\mathrm{tr}\left(J_2 A\right) = \mathrm{tr}\left(J_2 A'\right) = -\mathrm{tr}\left(A' J_2\right) = 0.$$

That is to say the only possible element in the invariant cone would be zero matrix, which does not suit our purpose. So J_2 can only be skew-symmetric.

Appendix B: Proof of the anticommutation relation between J_1 and J_2

Let A be any strict contractive element in the invariant cone with metric iJ_2, and $A' = i\left(A - \bar{A}\right)/2$. In this case $[J_2,\ A'] = 0$, and the real symmetric matrix $Q = J_2 A'$ is positive definite. We also have $\{J_1,\ A'\}= 0$, because $J_1^T A J_1 = \bar{A}$.

Now consider the real skew-symmetric matrix

$$X = -J_1 A' = J_1 J_2 Q = -Q J_2 J_1.$$

X has real orthogonal matrix $J_1 J_2$ and positive real symmetric matrix Q as its unique polar decomposition, which implies that $[J_1 J_2,\ Q] = 0$. Hence $\{J_1,\ J_2\}= 0$.