Semigroup approach to the sign problem in quantum Monte Carlo simulations

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We propose a framework based on the concept of the semigroup to understand the fermion sign problem. By using properties of contraction semigroups, we obtain 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 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 all the sign-problem-free fermion lattice models that 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 effectively getting numerical results for large systems at low temperature.

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 inverted temperature get larger[7, 8], 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[9], 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[10–12], the fermion bag[13, 14], the Majorana quantum Monte Carlo[15], the split orthogonal group[16], the Majorana reflection positivity[17], and the Majorana time-reversal symmetries[18]. Each approach has unified a class of sign-problem-free fermion models and brought additional examples of sign-problem-free QMC simulations.

In this work, we propose an alternative approach to construct fermion models without the sign problem. We observe that semigroup structures arise naturally from imaginary-time evolutions; this observation 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, then the QMC sampling weights are exactly the traces. This fact serves as the starting point of our approach.

A semigroup is a set with element multiplication that satisfies the associative law. Compared with the concept of a 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[19] is employed to study the time evolution of open quantum systems, where the concept of the semigroup reflects the irreversibility of time for the concerned physical processes. In quantum field theory and statistical physics, the renormalization group(RG)[20] 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 semigroup called the contraction semigroup. We construct two kinds of contraction semigroups. When the parameter region is contained in such semigroups, the fermionic Gaussian integral is always real non-negative. 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 framework. The Kramers time-reversal invariance leads to Kramers pairs of eigenvalues of matrices, which results in the non-negativity of
fermion determinants\[12\]. In Ref. [10], the relation be-
 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[17,18]. 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[17] is actually equivalent
to one of the two kinds of contraction semigroups treated
in this work. In short, to our best knowledge, all known
sign-problem-free fermion lattice models used in simu-
lation approaches based on semigroups can be understood
in our framework.

Our results open up new possibilities to sign-problem-
free Monte Carlo simulations. We construct a kind of in-
teracting fermion lattice model which involves the pairing
term, the Kramers time-reversal invariant hopping term,
and the interaction term. This class of model is sign-
problem-free, which could not be explained in previous
frameworks.

We believe that this framework will find more appli-
cations in both numerical and analytical studies[21]. 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, the fermionic operators are decoupled by auxiliary
fields into fermionic quadratic forms[5,6,22]. After in-
tegrating 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[10,23]

\[
p = \frac{\text{tr} (e^{h_1} e^{h_2} \cdots e^{h_k})}{\text{det} (I + e^{A_1} e^{A_2} \cdots e^{A_k})^{1/2}}. \tag{1}
\]

The expression of sampling weight in Eq. (1) is the
main object of study in this work. Here \( h_i = \gamma^T A_i \gamma / 4 \)
\((i = 1, \ldots, k)\) denotes 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. \( \gamma_n \) \((n = 1, \ldots, 2N)\)
are Majorana fermion operators, which satisfy the anti-
commutation relations \( \{ \gamma_i, \gamma_m \} = 2 \delta_{im} \). The Majorana
fermion basis is used for convenience; it is equivalent to
the complex fermion basis with \( N \) species. Unless we
specify a particular example, in principle \( h_i \) could con-
tain an arbitrary particle number conserving part and
an arbitrary pairing part. That is the equivalent of say-
ing that 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 cir-
cumstances, statistical sampling methods may fail to ob-
tain 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[24]. 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 semigroups.

Furthermore, if a Lie semigroup \( S \subseteq \text{Spin} (2N, \mathbb{C}) \)
has the property \( p \geq 0 \) for all its elements, then it corre-
sponds 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. [22,26].

For any square complex matrix \( X \), consider an anti-
linear symmetry operation \( X \mapsto \eta X^\dagger \eta \) given by a Her-
mitian matrix \( \eta = \eta^\dagger \) with \( \eta^2 = 1 \), together with Hermitian
conjugation. We say that the matrix is \( \eta \)-Hermitian or \( \eta \)-
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 prod-
ucts. Semigroups of this kind are called contraction semi-
groups. Equivalently, one can say that the contraction
semigroup consists of all the square matrices \( g \) that satis-
ify \( g^\dagger \eta g - \eta \leq 0 \). They contract the “length” of any
vector given by the metric \( \eta \). Similarly, one can define
the expansion semigroup by inverting the direction of the
inequality. We will work on the contraction semigroup
and leave the expansion case to the reader.

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

Specially, let us consider strict contraction elements,
which remain strict contractions when multiplied by any
semigroup elements. In the strict contraction case \( g^\dagger \eta g -
\( \eta < 0 \), which implies that \( \eta X_0 < 0 \) and \( g \) cannot have eigenvalues of magnitude 1. This means \( \det (I + g) \neq 0 \), which we use in the following section to construct sign-problem-free semigroups.

**IV. SIGN-PROBLEM-FREE SEMIGROUPS**

Let us give the outline of the discussions in this section. First, we restrict the range of parameters by an antilinear 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 nonstrict 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 antilinear 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.

First, we assume the complex skew-symmetric matrices are fixed under the operation \( A \mapsto J_1^T A J_1 \). Here \( J_1 \) could be either symmetric \( J_1^2 = I \) or skew-symmetric \( J_1^2 = -I \). It is easy to see that \( p \) is real under this assumption.

Second, to define a contraction semigroup, \( J_2 \) should be chosen to be either symmetric or skew-symmetric, so that \( J_2 \) or \( i J_2 \) can serve as the aforementioned indefinite metric \( \eta \). The coefficient matrices that are not changed under the transformation \( A \mapsto J_1^T A J_1 \) generate the maximal subgroup of the contraction semigroup. Meanwhile, elements in the invariant cone change sign under this operation, \( i J_2 A = -i A J_2 \leq 0 \). 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 satisfy 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 \( J_2 \). Under the current assumption, the only possibility is that \( J_1 \) and \( J_2 \) satisfy the anticommutation relation \( \{ J_1, J_2 \} = 0 \). See the Supplemental Material for more detailed arguments.

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

\[
J_1^T A J_1 = \bar{A}, \quad (2)
\]

\[
i \left( J_2 A - \bar{A} J_2 \right) \leq 0. \quad (3)
\]

### Table I. Classification of sign-problem-free quantum lattice fermion models.

| Cases | \( J_1^2 = I \), \( J_1^2 = -I \) | \( J_2^2 = I \), \( J_2^2 = -I \) |
|-------|---------------------------------|---------------------------------|
| \( J_1^2 \) \( \bar{A} \) \( J_2 \) | (a) | (b) |
| \( i \left( J_2 \bar{A} - \bar{A} J_2 \right) \leq 0 \) | (d) | (e) | (f) |

\( J_1 \) 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. Therefore, the condition for positive trace given above also holds for this complex orthogonal generalization of the Majorana fermion basis.

**V. APPLICATIONS**

Equations (2) and (3) constitute the main result of this work. They cover all the results on sign-problem-free QMC simulations of fermion lattice models known to us. They are classified and listed in Table I and are discussed type by type in this section.

First, when the inequality in Eq. (3) becomes equality, we will have two antilinear symmetries: \( J_1^T A J_1 = J_2^T A J_2 = A \). Under this circumstance our result goes back to the known results based on symmetry considerations. 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 the sign problem. For those models, \( J_1 \) could either be symmetric or skew-symmetric, due to the high symmetry of the systems.

(a) The negative-\( U \) Hubbard models, the positive-\( U \) Hubbard models at half-filling on bipartite lattices, and the Kane-Mele-Hubbard model at half-filling can all be regarded as good examples of this case. For those models, \( J_1 \) could be symmetric or skew-symmetric, due to the high symmetry of the systems.

(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 for the continuous-time quantum Monte Carlo (CTQMC) method. They have also been treated without the sign problem using the AFQMC method under the Majorana fermion basis, and using the CTQMC method under the framework of the split orthogonal group. Actually our result applies to several different kinds of QMC methods, such as CTQMC, despite their differences in practice. That class of spinless fermion models is made up of typical examples of the case with symmetric
(c) For the case with skew-symmetric $J_1$, the related fermion lattice models have Kramers time-reversal invariance \cite{17, 18}. Applications can also be found in high-spin interacting fermion systems, e.g., the nuclear shell model\cite{10} and the high-spin Hubbard model\cite{11, 12}. This sign-problem-free property of Kramers time-reversal model\cite{10}, and the high-spin Hubbard model\cite{11, 12}. This case has also been included in Theorem 2 of Ref. \cite{17}, where the matrices $A$, $J_2$, and $iJ_1J_2$ play the roles of $V$, $S$, and $P$ there, respectively.

Second, when the inequality in Eq. (3) is not an equality, parameters actually live in the whole semigroup. Models of this case can also be simulated by quantum Monte Carlo without the sign problem.

(d) We note that for some models, both symmetric and skew-symmetric $J_1$ are suitable. Those models correspond to the intersection of the two semigroups. A generalized Kane-Mele-Hubbard model with staggered magnetic field, considered in Ref. \cite{17}, can be seen as an example.

(e) When $J_1$ is symmetric, the parameter region given by Eqs. (2) and (3) coincides with the result obtained from Majorana reflection positivity. To see this clearly, one may choose a Majorana fermion basis such that $J_1 = \sigma_1 \otimes I_N$ and $J_2 = i \sigma_2 \otimes I_N$. 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 $\gamma^T A \gamma = \gamma^{(1)} B \gamma^{(1)} + \gamma^{(2)} B \gamma^{(2)} + 2 \gamma^{(1)} C \gamma^{(2)}$, with block matrices $B$ and $C$. $C$ is positive semidefinite Hermitian matrix. This can be immediately compared to the related definitions in Ref. \cite{17}. 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 operator multiplication\cite{17, 33}, which accounts for 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\cite{38, 40}.

(f) When $J_1$ is skew-symmetric, the result in the previous section 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 the 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 $J_1 = \sigma_x \otimes i \sigma_y \otimes I_{N/2}$ and $J_2 = -i \sigma_y \otimes I_2 \otimes I_{N/2}$. Then we define the complex fermion basis as $c_l = (\gamma^{(1)}_l + i \gamma^{(2)}_l)/2$ and $d_l = (\gamma^{(4)}_l + i \gamma^{(3)}_l)/2$, where $l = 1, \ldots, N/2$ 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,

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

$$h^{(0)} = (c^\dagger, d^\dagger) M (c, d) M^T (c^\dagger, d^\dagger),$$

$$h^{(p)} = (c, d) R K \frac{1}{4} (\gamma^T A \gamma) (c^\dagger, d^\dagger).$$

Here, $M, R$, and $S$ are complex coefficient matrices, and $K = i \sigma_y \otimes I_{N/2}$. $R K$ and $S K$ are skew-symmetric, in accordance with the fermion anticommutation relations.

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\cite{11}, sign-problem-free AFQMC simulations can be carried out for this type of model\cite{12}. Now we can extend this model by adding a new pairing term that 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.

As an example of this case, consider the model Hamiltonian $H = H_0 + H_1 + H_p + H_U$ defined on a square
lattice, where

\[ H_0 = -t \sum_{\langle i,j \rangle} (c_i^+ c_j + h.c.) - t \sum_{\langle i,j \rangle} (d_i^+ d_j + h.c.) , \]  

(7)

\[ H_\perp = -t_\perp \sum_i ( -1 )^{x_i + y_i} (c_i^+ d_i + h.c.) , \]  

(8)

\[ H_p = \sum_i [ \Delta (c_i^+ d_{i+\delta_x} - c_i^+ d_{i+\delta_y} + c_i^+ d_{i-\delta_x} - c_i^+ d_{i-\delta_y}) + h.c.] , \]  

(9)

\[ H_U = U \sum_i \left( c_i^+ c_i - \frac{1}{2} \right) \left( d_i^+ d_i - \frac{1}{2} \right) . \]  

(10)

Here \( t, t_\perp, \) and \( U \) are real parameters, \( U \geq 0 \), and \( \Delta \) is a complex parameter. Here \( H_1 \) describes the effect of a staggered magnetic field along the \( x \) axis, and \( H_p \) describes the \( d \)-wave BCS pairing. The whole Hamiltonian depicts the proximity effect between superconductivity and antiferromagnetism and can be simulated by the AFQMC method without the sign problem. This can be proved by introducing the particle-hole transformation \( d_i \rightarrow ( -1 )^{x_i + y_i} d_i^+ \) and suitable HS transformations. When \( t_\perp = 0 \), the single-body term of the Hamiltonian is gapless and the whole Hamiltonian has been used to study the quantum criticality of the chiral Heisenberg universality class. When \( t_\perp \neq 0 \), the whole Hamiltonian exhibits a single-particle gap.

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 the 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

\[ \text{tr} ( h_1^g h_2^g \ldots h_m^g g_0 ) \geq 0, \]  

(11)

where the coefficient matrices of fermionic quadratic operators \( h_i^g \) belong to the invariant cone, \( s = 1, \ldots, m \), and \( g_0 \) can take any elements of the semigroup. The proof is straightforward for the case with symmetric \( J_1 \) owing to Majorana reflection positivity. A proof for the case with skew-symmetric \( J_1 \) using Wick’s theorem and the Kramers degeneracy theorem can be found in the Supplemental Material. This set of inequalities also provides an alternative route to the sign-problem-free property. They are also very useful when considering the sign problem in zero temperature AFQMC simulations.

VI. CONCLUSION AND DISCUSSION

In this work we have presented sufficient conditions for sign-problem-free QMC simulations of fermion lattice models. A framework based on the concept of the semigroup has been proposed to understand this problem in a systematic way. Sufficient conditions have been obtained, as stated in Eqs. (2) and (3). All previous results based on symmetry considerations and Majorana reflection positivity can be understood well and unified naturally within our approach. Alternative 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.

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 $A' = \left( A + A^T \right)/2$. From $J_2^2 A J_2 = -A$ we know that $\{ J_2, A' \} = 0$. Then we would have

$$\text{tr} (J_2 A) = \text{tr} (J_2 A') = -\text{tr} (A' J_2) = 0.$$ 

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 contraction element in the invariant cone with metric $i J_2$, and $A' = i (A - A^T)/2$. In this case $[J_2, A'] = 0$. We also have $\{ J_1, A' \} = 0$, because $J_1^2 A J_1 = A$. We can always select an $A$ such that the real symmetric matrix $Q = -J_2 A'$ is positive definite.

Now consider the real symmetric (when $J_1^2 = I_{2N}$) or skew-symmetric (when $J_1^2 = -I_{2N}$) 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 $\{ J_1, J_2 \} = 0$.

Appendix C: Proof of a series of trace inequalities

Now we prove the inequality in Eq. (11) of the main text for the case with skew-symmetric $J_1$. To this purpose, we show an equivalent result that any trace with the form

$$W = (-1)^r \text{tr} \{ f_4 r f_4 r - 1 \ldots f_2 s f_2 s - 1 \ldots f_2 f_1 \exp (h) \}$$

is non-negative for any positive integer $r$, where $h$ can take any particle number conserving fermionic quadratic forms with Kramers time-reversal invariance. $f_{2s-1} (s = 1, \ldots, 2r)$ can take any fermion annihilation or creation operators (which we do not require to form an orthogonal basis), while $f_{2r}$ are their images under the time-reversal operation respectively.

Let $Z = \text{tr} \{ \exp (h) \} \geq 0$ and assume $Z \neq 0$ so that the Green’s function $G$ can be defined by

$$G_{ij} = -\frac{1}{Z} \text{tr} \{ \theta (i - j) f_i f_j - \theta (j - i) f_j f_i \exp (h) \}$$

with $i, j = 1, \ldots, 4r$, and $\theta$ is the unit step function. Only the contractions between annihilation and creation operators lead to non-zero elements of $G$. Define the skew-symmetric matrix $\tilde{G}$ by $\tilde{G}_{ij} = G_{ij}$ when $i > j$. In the non-trivial case there are $2r$ creation operators and $2r$ annihilation operators in total. Therefore one can select an appropriate permutation matrix $P$ such that

$$\tilde{G} = P^T \begin{pmatrix} 0 & M \\ -M^T & 0 \end{pmatrix} P$$

with $\det P = 1$, meanwhile the Kramers time-reversal symmetry leads to the relation

$$J_M^T M J_M = \tilde{M},$$

where $J_M$ is a skew-symmetric real orthogonal matrix. So all the eigenvalues of $M$ occur in complex conjugate pairs even when they are real numbers, which is ensured by the Kramers degeneracy theorem.

By Wick’s theorem we have the Pfaffian expression for the expectation

$$W = \frac{(-1)^r}{(2r)! 4^r} \text{pf} (\tilde{G}) Z = \frac{1}{(2r)! 4^r} \det (M) Z,$$

which is clearly non-negative.