## <span id="page-0-1"></span>Majorana-Time-Reversal Symmetries: A Fundamental Principle for Sign-Problem-Free Quantum Monte Carlo Simulations

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A fundamental open issue in physics is whether and how the fermion sign problem in quantum Monte Carlo (QMC) simulations can be solved generically. Here, we show that Majorana-time-reversal (MTR) symmetries can provide a unifying principle to solve the fermion sign problem in interacting fermionic models. By systematically classifying Majorana-bilinear operators according to the anticommuting MTR symmetries they respect, we rigorously prove that there are two and only two *fundamental* symmetry classes which are sign-problem-free and which we call the "Majorana class" and "Kramers class," respectively. Novel sign-problem-free models in the Majorana class include interacting topological superconductors and interacting models of charge- $4e$  superconductors. We believe that our MTR unifying principle could shed new light on sign-problem-free QMC simulation on strongly correlated systems and interacting topological matters.

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Interactions between particles are ubiquitous, and studying interacting models of many-body systems is of central importance in modern condensed matter physics [\[1](#page-4-1)–3], quantum chromodynamics, and other fields. However, almost all interacting models in two and three dimensions, especially those with strong correlations, are beyond the solvability of any known analytical methods. Consequently, developing efficient and unbiased numerical methods plays a key role in understanding many-body physics in solid state materials like high-temperature superconductors [\[4,5\]](#page-4-2) and other systems such as quark matter. Quantum Monte Carlo (QMC) simulation is among the most important approaches to study interacting manybody systems [6–[21\],](#page-4-3) as it is numerically exact and intrinsically unbiased. Nonetheless, QMC simulation often encounters the notorious fermion sign problem, making it practically infeasible to study those models with large sizes and at a low temperature [\[22\]](#page-4-4). It has been highly desired to find solutions to the fermion sign problem in interesting models that are relevant to intriguing systems such as hightemperature superconductors [\[23\]](#page-4-5).

Even though a general solution of the fermion sign problem is nondeterministic polynomial hard [\[24\]](#page-4-6), many specific interacting models have been successfully identified to be sign-problem-free. One prototype sign-problemfree example is the repulsive Hubbard model at half filling [\[8\]](#page-4-7). In the language of auxiliary-field QMC simulation [\[6](#page-4-3)–8], the partition function  $Z = \sum \rho$ , where the Boltzmann weight  $\rho = \text{Tr} \prod_{i=1}^{N_{\tau}} \exp[\hat{h}_i]$  with  $\hat{h}_i$  being fermion-bilinear operators depending on auxiliary fields Bonzinalin weight  $p = \prod_{i=1}^n \exp[n_i]$  with  $n_i$  being<br>fermion-bilinear operators depending on auxiliary fields at imaginary time  $\tau_i$ . If all Boltzmann weight  $\rho > 0$ , the simulation is free from the fermion sign problem, and the needed computation time grows only polynomially with the system size. Tremendous effort has been devoted to construct a fundamental principle for solving the fermion sign problem.

One successful strategy of solving the sign problem is to employ the Kramers symmetry of fermion-bilinear operators  $\hat{h}_i$ , which is defined as having both time-reversal symmetry  $\hat{\Theta}$  with  $\hat{\Theta}^2 = -1$  and charge conservation  $\hat{Q}$ . With the Kramers symmetry, eigenvalues always appear in Kramers pairs such that the Boltzmann weight can be shown to be positive definite [\[25\]](#page-4-8). Sign-problem-free models with Kramers symmetry have been studied

<span id="page-0-0"></span>TABLE I. The "periodic table" of sign-problem-free symmetry classes defined by the set of anticommuting Majorana-timereversal symmetries  $\{T_1^{p_1}, T_2^{p_2}, ..., T_n^{p_n}\}$  they respect, where  $p_i = +$  and  $(T^{\pm})^2 = +1$  We rigorously proved that there are two and  $\pm$  and  $(T_i^{\pm})^2 = \pm 1$ . We rigorously proved that there are two and only two *fundamental* symmetry classes which are sign-problemonly two fundamental symmetry classes which are sign-problemfree: the Majorana class and Kramers class, respectively. For the former, Majorana-bilinear operators possess two MTR symmetries  $T_1^+$  and  $T_2^-$  with  $T_1^+ T_2^- = -T_2^- T_1^+$ , and it is a *genuinely*<br>new sign-problem-free symmetry class introduced in Ref. [26] new sign-problem-free symmetry class introduced in Ref. [\[26\],](#page-4-9) qualitatively different from the latter, which is based on the conventional Kramers-time-reversal symmetry studied in Ref. [\[25\].](#page-4-8)



extensively during the past three decades. One naturally asks if a more fundamental symmetry principle exists for solving the fermion sign problem in models whose signproblem solutions remain unknown so far.

Recently, Majorana representation was first introduced by three of us in Ref. [\[26\]](#page-4-9) to solve the fermion sign problem in models (including spinless and spinful fermion models) which are beyond the Kramers method. Here we employ time-reversal symmetry in Majorana representations [\[26\]](#page-4-9) as a fundamental and unifying principle to solve the fermion sign problem. We first classify Majorana-bilinear operators  $h = \gamma^{T} h \gamma$  according to their Majorana-time-reversal (MTR) symmetries, where  $h^T = -h$  is an antisymmetric matrix and  $\gamma^T = (\gamma_1, ..., \gamma_{2N})$  are Majorana operators with  $\{\gamma_i, \gamma_j\} = 2\delta_{ij}$  [\[27\],](#page-4-10) and then identify all symmetry classes which must be sign-problem-free. Note that "time reversal" here generally represents "antiunitary." Because Majorana operators are real, Majorana-time-reversal transformation can be represented by  $T = UK$ , where U are real orthogonal matrices and K is complex conjugation with  $T^2 = \pm 1$ for  $U^T = \pm U$ . By systematically classifying Majoranabilinear operators according to the maximal set of anticommuting MTR symmetries they respect, we prove that there are only two fundamental symmetry classes of models which are sign-problem-free: the Majorana class and Kramers class, respectively. Other sign-problem-free symmetry classes have higher symmetries than the two fundamental ones, as shown in Table [I.](#page-0-0)

For the Majorana class, the Majorana-bilinear operators possess two anticommuting symmetries  $T_1^+$  and  $T_2^-$ , where  $(T_i^{\pm})^2 = \pm 1$ . Majorana-bilinear operators in this class can<br>always be transformed into two decoupled parts which are always be transformed into two decoupled parts which are time-reversal partners to each other such that it is signproblem-free [\[26\]](#page-4-9). For the Kramers class, from anticommuting  $T_1^-$  and  $T_2^-$ , the usual Kramers-time-reversal symmetry can be identified so that they are sign-problem-free. Recently, various correlated models in the Kramers class were studied by QMC simulation to investigate high-temperature superconductivity near quantum critical points (QCPs) [\[28](#page-4-11)–34].

It is worth pointing out that sign-problem-free models in the genuinely new Majorana class include interacting topological superconductors with helical Majorana edge states [35–[37\]](#page-4-12) and the minimal model for charge-4e superconductors [\[38\]](#page-4-13). Note that the sign problems of these models are beyond applicability of other known approaches, especially those requiring particle-number conservation [\[39,40\]](#page-4-14). In contrast, the Majorana approach here is general and can be applied to generic models whether the particle number is conserved or not. As an application of our Majorana approach, we have performed large-scale sign-problem-free Majorana QMC simulations on interacting time-reversal-invariant topological  $p + ip$ superconductors of spin- $1/2$  electrons and found that with increasing interactions the system encounters a quantum phase transition from a topological nontrivial superconducting phase to a topologically trivial one by spontaneously breaking time-reversal symmetry [\[41\]](#page-4-15). To the best of our knowledge, it is the first time that a topological quantum phase transition of spontaneous time-reversal symmetry in superconductors can be studied by numerically exact and intrinsically unbiased simulations.

Majorana-time-reversal symmetry classes.—Timereversal symmetry plays an important role in classifying random matrices as well as topological insulators or superconducutors [\[42](#page-4-16)–46] and in avoiding the fermion sign problem in QMC simulations [\[25\].](#page-4-8) The Kramers-timereversal symmetry [\[25\]](#page-4-8) has been a successful guiding principle for sign-problem-free QMC simulations. Nonetheless, it requires particle-number conservation and is then not the most general time-reversal symmetry one can utilize to prevent the fermion sign problem [\[26\]](#page-4-9). Thus, constructing a more fundamental and generic symmetry principle to avoid the fermion sign problem is desired.

<span id="page-1-0"></span>In Ref. [\[26\]](#page-4-9) we proposed that time-reversal symmetry in the Majorana representation can be used to avoid the sign problem in interacting models. Namely, one can employ Majorana fermions to write fermion-bilinear operators:  $\hat{h}(\tau_i) \equiv \hat{h}_i = \gamma^T h_i \gamma$ , where  $\gamma^T = (\gamma_1^1, ..., \gamma_N^1, \gamma_1^2, ..., \gamma_N^2)$ <br>and h; is a 2N × 2N matrix. In the case that and  $h_i$  is a  $2N \times 2N$  matrix. In the case that

$$
h_i = \begin{pmatrix} B_i & 0 \\ 0 & B_i^* \end{pmatrix}, \tag{1}
$$

 $\rho = \text{Tr} \prod_{i=1}^{N_{\tau}} \exp[\hat{h}_i]$  is positive definite because of the Majorana-time-reversal symmetry  $T^+ - \tau^X K$  under which  $\varphi = \pi \prod_{i=1}^{\infty} \exp[n_i]$  is positive definite because of the<br>Majorana-time-reversal symmetry  $T^+ = \tau^x K$ , under which<br> $\tau^1 \to \tau^2$ ,  $\tau^2 \to \tau^1$  and  $R \to R^*$  [26]. Here  $\tau^{\alpha}$  are Pauli  $\gamma_i^1 \rightarrow \gamma_i^2$ ,  $\gamma_i^2 \rightarrow \gamma_i^1$ , and  $B_i \rightarrow B_i^*$  [\[26\].](#page-4-9) Here  $\tau^{\alpha}$  are Pauli matrices acting in the Majorana space (1, 2). Because no coupling between  $\gamma^1$  and  $\gamma^2$  exists in  $\hat{h}_i$ , tracing over the Hilbert space of  $\gamma^1$  and  $\gamma^2$  can be done separately and  $\rho_2 =$  $\rho_1^*$  due to the Majorana-time-reversal symmetry such that  $\rho = \rho_1 \rho_2 > 0$ .

Note that  $h_i$  in Eq. [\(1\)](#page-1-0) also respects another Majoranatime-reversal symmetry  $T^- = i\tau^{\gamma}K$ , besides  $T^+ = \tau^{\gamma}K$ . Moreover,  $T^+T^+ = -T^+T^-$ . One naturally asks the following question: Can any Majorana-bilinear operator respecting anticommuting  $T^+$  and  $T^-$  symmetries be transformed into the form in Eq. [\(1\)](#page-1-0) such that it is sign-problem-free? The answer is positive, as shown below. This further motivates us to ask another question: Can anticommuting Majorana-time-reversal symmetries provide a fundamental principle to classify Majorana-bilinear operators such that general sufficient conditions for sign-problem-free models can be constructed? Our answer is also positive, as we prove below.

As Majorana fermion operators are real, Majorana-timereversal symmetry can be represented by  $T^{\pm} = U^{\pm} K$ , where  $(T^{\pm})^2 = \pm 1$  and  $U^{\pm}$  is a real orthogonal matrix satisfying  $(U^{\pm})^T = \pm U^{\pm}$ . We propose to systematically classify generic Majorana-bilinear operators  $\hat{h}_i$  according

to the maximal set of anticommuting MTR symmetries  $C = \{T_1^{p_1}, ..., T_n^{p_n}\}\$  they respect, namely,  $[T_j^{p_j}, h_i] = 0$  and  $T_j^{p_j} \cdot T_j^{p_j} \cdot T_j^{p_j}$  $T_i^{p_i}T_j^{p_j}+T_j^{p_j}T_i^{p_i}=p_i2\delta_{ij}$ , where  $p_i=\pm$ . Because of the sign choices of  $p_i = \pm$ , there are totally  $n + 1$  distinct symmetry classes for each *n*. For  $n = 0$ , there is only one symmetry class  $\{I\}$ , which means that no Majorana-timereversal symmetry can be found for those Majoranabilinear operators; while for  $n = 1$  there are two symmetry classes:  $\{T_1^+\}$  and  $\{T_1^-\}$ . For  $n = 2$  we have three sym-<br>metry classes:  $\{T^+$   $T^+\}$   $\{T^+$   $T^-$  and  $\{T^ T^-$ ). Here metry classes:  $\{T_1^+, T_2^+\}, \{T_1^+, T_2^-\}, \text{ and } \{T_1^-, T_2^-\}.$  Here,<br>we are concerned with only the symmetries of h,: namely we are concerned with only the symmetries of  $h_i$ ; namely, we assume that  $h_i$  are random matrices except respecting the specified set of anticommuting MTR symmetries. This classification scheme using anticommuting symmetries is, in spirit, similar to the one employed by Kitaev using the Clifford algebra to classify random matrices and construct the periodic table of topological insulators and superconductors [\[44\].](#page-4-17)

Obviously, if a symmetry class  $C$  is sign-problem-free, any higher symmetry class  $\mathcal{C}'$  whose symmetries can generate all the symmetries of  $C$  must be sign-problemfree. For instance, the symmetry class  $\{T_1^+, T_2^+, T_3^+, T_4^+\}$  is<br>bigher than the symmetry class  $\{T_1^+, T_2^-\}$  because  $T_2^-$  in higher than the symmetry class  $\{T_1^+, T_2^-\}$ , because  $T_2^-$  in<br>the latter can be generated from the former by identifying the latter can be generated from the former by identifying  $T_2^2 = T_2^2 T_3^2 T_4^4$ . If the former is sign-problem-free, the latter must be sign-problem-free. Consequently, it would be latter must be sign-problem-free. Consequently, it would be sufficient to derive all the fundamental symmetry classes which are sign-problem-free.

"Periodic table" of fermion sign problem.—It was known that the fermion sign problem can appear in the following three symmetry classes:  $\{I\}$ ,  $\{T_1^+\}$ , and  $\{T_1^-\}$ , as<br>sign-problematic examples in these three symmetry classes sign-problematic examples in these three symmetry classes are known. For instance, Tr  $\exp[x\gamma^1\gamma^2] = 2\cos x$ , which is<br>negative for  $x \in (\frac{\pi}{2}, \pi)$  even though the Majorana-bilinear negative for  $x \in (\frac{\pi}{2}, \pi)$ , even though the Majorana-bilinear<br>operator  $xy^1y^2$  respects the T<sup>-</sup> symmetry  $(y^1 \rightarrow y^2)$ operator  $xy^1y^2$  respects the  $T_1^-$  symmetry  $(y^1 \rightarrow y^2)$ ,  $\gamma^2 \rightarrow -\gamma^1$ , plus complex conjugation). This illustrates that the symmetry of  $T_1^-$  cannot guarantee sign-problem-free. Consequently, symmetry itself for these classes  $\{I\}$ ,  $\{T_1^+\}$ ,  $\{T_2^-\}$  is not sufficient to guarantee the absence of the sign  ${T_1 \choose T_1}$  is not sufficient to guarantee the absence of the sign<br>problem. We then move to symmetry classes with  $n = 2$ problem. We then move to symmetry classes with  $n = 2$ anticommuting symmetries:  $\{T_1^+, T_2^+\}, \{T_1^+, T_2^-\},$  and  $\{T_1^-, T_2^-\}$  and  $\{T_1^-, T_2^+\}$  cannot  ${T_1, T_2}$ . The symmetries in the class  ${T_1^+, T_2^+}$  cannot<br>guarantee sign-problem-free because there are known guarantee sign-problem-free, because there are known examples with the fermion sign problem in this class, as shown explicitly below. How about the other two classes  $\{T_1^+, T_2^-\}$  and  $\{T_1^-, T_2^-\}$ ? It turns out these two are fundamental symmetry classes which are sign-problemfundamental symmetry classes which are sign-problemfree, as we shall prove below.

If Majorana-bilinear operators  $\hat{h}_i$  respect MTR symmetries in one of the two symmetry classes  $\{T_1^+, T_2^-\}$  and  $\{T^-, T^-\}$   $q = \text{Tr} \prod^{N_z} \exp[\hat{h}_z] > 0$ . These two are the only  ${T_1^-, T_2^-, \rho = \text{Tr} \prod_{i=1}^{N_{\tau}} \exp[\hat{h}_i] > 0.$  These two are the only fundamental symmetry classes which are sign-problem- $\{I_1, I_2\}$ ,  $\rho = \Pi \prod_{i=1}^{\infty} \exp[i_i] > 0$ . These two are the only fundamental symmetry classes which are sign-problemfree. We shall prove this below for the two symmetry classes separately. We call the former symmetry class as the Majorana class, while the latter one as Kramers class for reasons which will be clear later.

Majorana class.—In the Majorana class, the random matrix  $h_i$  respects two Majorana-time-reversal symmetries  $T_1^+ = U_1^+ K$  and  $T_2^- = U_2^- K$ , where  $U_1^+$  is a real-symmetric<br>orthogonal matrix but  $U_2^-$  a real antisymmetric orthogonal orthogonal matrix but  $U_2^-$  a real antisymmetric orthogonal matrix. From these two time-reversal symmetries, one can construct a unitary symmetry  $P = T_1^+ T_2^- = U_1^+ U_2^-$ . It is<br>straightforward to see that P is a real symmetric matrix straightforward to see that  $P$  is a real symmetric matrix satisfying  $P^2 = 1$ . Consequently, the eigenvalues of P are  $\pm 1$ . As  $[P, h_i] = 0$ , we can use P to block-diagonalize  $h_i$ .<br>We denote the eigenvectors of P with eigenvalue +1 as

We denote the eigenvectors of P with eigenvalue  $+1$  as  $\chi_a$ , namely,  $P\chi_a = \chi_a$ , where  $a = 1, ..., N$ . Because P is a real-symmetric matrix,  $\chi_a$  can be chosen to be real, i.e.,  $\chi_a^* = \chi_a$ . Since  $T_1^+$  satisfies  $\{T_1^+, P\} = 0$ ,  $T_1^+ \chi_a$  are eigen-<br>vectors of P with eigenvalue  $-1$ . Now we are ready to vectors of  $P$  with eigenvalue  $-1$ . Now, we are ready to use the basis  $\tilde{\chi} = (\chi_1, ..., \chi_N, T_{1}^{+}\chi_1, ..., T_{1}^{+}\chi_N)$  to block-<br>diagonalize the 2N × 2N matrix h, as follows: diagonalize the  $2N \times 2N$  matrix  $h_i$ , as follows:

$$
\tilde{\chi}^T h_i \tilde{\chi} = \begin{pmatrix} B_i & 0 \\ 0 & B_i^* \end{pmatrix} . \tag{2}
$$

Consequently, the Boltzmann weights  $Tr \prod_{i=1}^{N_{\tau}} exp[\hat{h}_i]$  are nositive definite as required by the time-reversal symmetry Consequently, the Bonzmann weights  $\Pi \prod_{i=1} exp[n_i]$  are positive definite, as required by the time-reversal symmetry between the two decoupled blocks  $B_i$  and  $B_i^*$ . Because charge conservation is not required for this symmetry class of  $\{T_1^+, T_2^-\}$ , it is a new *sign-problem-free* symmetry class<br>which was first studied in Ref. [26]. We call it the which was first studied in Ref. [\[26\].](#page-4-9) We call it the Majorana class.

*Kramers class.*—From  $T_1^-$  and  $T_2^-$  symmetries, a unitary symmetry  $Q = T_1^T T_2^-$  can be derived. Because Q is anti-<br>symmetric, namely  $Q^T = -Q$  one can construct a charge symmetric, namely,  $Q^T = -Q$ , one can construct a charge operator  $\hat{Q} = \gamma^T (i\hat{Q})\gamma$  such that  $[\hat{Q}, \hat{h}_i] = 0$ . It is clear that the combination of  $T^-$  and  $Q$  charge conservation in this because  $Q = \gamma$  ( $Q/\gamma$  such that  $Q, n_i$ ) = 0. It is clear that the combination of  $T_1^-$  and Q charge conservation in this symmetry class is equivalent to the Kramers symmetry, since  $[T_1^-, iQ] = 0$  and  $(T_1^-)^2 = -1$ . The absence of the fermion sign problem has been shown in Ref. [25] accordfermion sign problem has been shown in Ref. [\[25\]](#page-4-8) according to the observation of the Kramers pairs in eigenvalues. Because of the Kramers symmetry, we denote this symmetry class as the Kramers class.

For symmetry classes with  $n \geq 3$ , it turns out that all of them, except only one class  $\{T_1^+, T_2^+, T_3^+\}$ , can generate the<br>symmetries in either the Majorana class or the Kramers symmetries in either the Majorana class or the Kramers class. For instance, the symmetry class  $\{T_1^+, T_2^+, T_3^-\}$  has<br>higher symmetry than  $\{T^+, T^- \}$  and  $\{T^+, T^- - T^-\}$  higher higher symmetry than  $\{T_1^+, T_2^-\}$  and  $\{T_1^+, T_2^-, T_3^-\}$  higher<br>than both  $\{T^+$ ,  $T^-$  and  $\{T^-$ ,  $T^-$  lacktriangle remaining than both  $\{T_1^+, T_2^-\}$  and  $\{T_1^-, T_2^-\}$ . The only remaining<br>unclear class is  $\{T^+ \mid T^+ \}$  which cannot generate unclear class is  $\{T_1^+, T_2^+, T_3^+\}$ , which cannot generate  $\{T^+$ ,  $T^-$  }  $T^ T^-$  }. Even though the symmetry class  $\{T_1^+, T_2^-\}$  or  $\{T_1^-, T_2^-\}$ . Even though the symmetry class  $\{T_1^+, T_2^+\}$  has relatively high symmetries it can still  $\{T_1^+, T_2^+, T_3^+\}$  has relatively high symmetries, it can still<br>suffer from the fermion sign problem, as we show below suffer from the fermion sign problem, as we show below that there exist explicit examples in this symmetry class which are sign-problematic.

Now we explicitly demonstrate that the two symmetry classes  $\{T_1^+, T_2^+\}$  and  $\{T_1^+, T_2^+, T_3^+\}$  can be sign-problem-<br>atic by considering the spin-1 repulsive Hubbard model atic by considering the spin- $\frac{1}{2}$  repulsive Hubbard model

away from half filling as an example. For the repulsive-U Hubbard model

$$
H = -t\sum_{\langle ij\rangle\sigma} [c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.}] + U\sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma}, \quad (3)
$$

where  $U > 0$ ,  $\mu \neq 0$ , and  $\sigma = \uparrow, \downarrow$ , we obtain the following decoupled Majorana-bilinear Hamiltonian  $\hat{h}_n$ after utilizing the Majorana representations  $c_{\sigma} = (\gamma_{\sigma}^1 +$ after utilizing the Majorana representations  $c_{\sigma} = (r_{\sigma} + i r_{\sigma}^2)/2$  and performing a Hubbard-Stratonovich (HS)<br>transformation:  $\hat{h} = -(\tilde{t}/2)\sum_{\mu\nu} x_{\mu}^T \sigma^0 \tau^y x_{\nu} + \sum_{\nu} [(\tilde{u}/2)]^2$ transformation:  $\hat{h}_n = -(\tilde{t}/2) \sum_{\langle ij \rangle} \gamma_i^T \sigma^0 \tau^y \gamma_j + \sum_i [(\tilde{\mu})^T \sigma^0 \tau^y \gamma_x - \lambda \sigma^0 \tau^y \tau^z \gamma_x]$  where  $\sigma^n$  are auxiliary fields  $4\gamma_i^T \sigma^0 \tau^y \gamma_i - \lambda \phi_i^p \gamma_i^T i \sigma^y \tau^z \gamma_i$ , where  $\phi_i^{\mu}$  are auxiliary fields<br>on site *i* at imaginary time  $\tau \gamma_i^T = (\gamma_1^1, \gamma_1^1, \gamma_2^2, \gamma_3^2, \gamma_4^2)$  is on site *i* at imaginary time  $\tau_n$ ,  $\gamma_i^T = (\gamma_{i\uparrow}^1, \gamma_{i\downarrow}^1, \gamma_{i\uparrow}^2, \gamma_{i\downarrow}^2)$ ,  $\sigma^a$  is Pauli matrix in spin space and  $\tau^a$  in Majorana space [411] It is Pauli matrix in spin space and  $\tau^a$  in Majorana space [\[41\].](#page-4-15) It is straightforward to show that  $\hat{h}_n$  possesses three MTR symmetries  $T_1^+ = \sigma^x \tau^x K$ ,  $T_2^+ = \sigma^z \tau^x K$ , and  $T_3^+ = \sigma^0 \tau^z K$ . Even though respecting these symmetries, the appearance of the sign problem in this decoupled channel for the doped repulsive Hubbard model is well known. In order to further confirm it, we have also computed the Boltzmann weights for different auxiliary-field configurations and find that negative weights can indeed appear. Namely, models in the symmetry class  $\{T_1^+, T_2^+, T_3^+\}$  can be sign-problematic. Since the class  $\{T_1^+, T_2^+, T_3^+\}$  has bigher sign-problematic. Since the class  $\{T_1^+, T_2^+, T_3^+\}$  has higher<br>symmetries than  $\{T_1^+, T_2^+\}$  the latter is also signsymmetries than  $\{T_1^+, T_2^+\}$ , the latter is also sign-<br>problematic problematic.

Combining the results above, we have shown that there are two and only two fundamental sign-problem-free symmetry classes: the Majorana class and the Kramers class. The periodic table of symmetry classes which are sign-problem-free or sign-problematic is shown in Table [I](#page-0-0). It provides a fundamental principle to identify sign-problem-free interacting fermion models.

Interacting topological superconductors in the Majorana class.—So far, novel interaction effects in topological superconductors have not been investigated by large-scale QMC simulation mainly due to the lack of such sign-problem-free models, although interacting topological insulators have been much studied by sign-problem-free QMC simulations [47–[54\].](#page-5-0) As mentioned above, there is no requirement of charge conversation for models in the Majorana class. Consequently, interesting sign-problem-free models describing interacting superconductors may be identified in this class such that we can study a strong correlation effect in superconductors using sign-problem-free QMC simulations. Indeed, we have found interacting models of topological superconductors with helical Majorana edge states which are sign-problem-free in the Majorana class.

<span id="page-3-0"></span>We first consider the Hamiltonian describing a topological superconductor of spin- $1/2$  electrons on the square lattice with time-reversal symmetry:

$$
H = \sum_{ij,\sigma} [-t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma} + \Delta_{ij,\sigma}c_{i\sigma}^{\dagger}c_{j\sigma}^{\dagger} + \text{H.c.}] - U \sum_{i} n_{i\uparrow}n_{i\downarrow},
$$
\n(4)

where  $c_{i\sigma}^{\dagger}$  creates spin-1/2 electrons with spin polarization  $\sigma = \uparrow, \downarrow, n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}, t_{ij} = t$  is nearest-neighbor hopping,<br>and  $t_{\uparrow} = u$  is the chemical notential. When  $\Delta_{\uparrow} = \Delta$  for and  $t_{ii} = \mu$  is the chemical potential. When  $\Delta_{ii,\sigma} = \Delta$  for  $j = i + \hat{x}$  and  $\Delta_{ij,\sigma} = i\sigma\Delta$  for  $j = i + \hat{y}$ , the Hamiltonian in Eq. [\(4\)](#page-3-0) describes a helical topological superconductor [\[44](#page-4-17)–46] with  $(p + ip)$  triplet pairing of spin-up electrons and  $(p - ip)$  triplet pairing of spin-down electrons, which hosts helical Majorana edge states protected by the Majorana-time-reversal symmetry  $T^- = i\sigma^y\tau^zK$ , where  $\sigma^i$ acts in spin space and  $\tau^i$  in the Majorana space. Besides  $T^-,$ it also possesses a unitary symmetry  $P = \sigma^z$ , such that we<br>can construct another Majorana-time-reversal symmetry can construct another Majorana-time-reversal symmetry  $T^+ = PT^- = \sigma^x \tau^z K$ . In the complex fermions basis, these<br>two anticommuting TR symmetries are  $T^+ = \sigma^x K$  and two anticommuting TR symmetries are  $T^+ = \sigma^x K$  and  $T^- = i\sigma^y K$ , where  $\sigma^a$  is the Pauli matrix acting in spin space  $(c<sub>↑</sub>, c<sub>↓</sub>)$ . Note that the unitary symmetry  $P = \sigma^z$  is not a  $U(1)$  symmetry conserving the total  $S^z$ , because the triplet pairing in the Hamiltonian breaks the U(1) symmetry. Instead, it conserves only the spin parity  $(-1)^{N_{\downarrow}}$ , where  $N_{\perp}$  is the number of spin-down electrons. The topological classification of superconductors respecting the time-reversal symmetry and the spin-parity symmetry in the noninteracting limit is  $\mathbb{Z}$ . In the presence of interactions, its topological classification was shown to be  $\mathbb{Z}_8$  [35–[37\].](#page-4-12)

For the Hubbard interactions, we perform the following HS transformation:

$$
e^{(U/4)\Delta\tau i\gamma_{i\uparrow}^1\gamma_{i\uparrow}^2 i\gamma_{i\downarrow}^1\gamma_{i\downarrow}^2} = \sum_{\phi_i=\pm 1} A e^{\lambda \phi_i (i\gamma_{i\uparrow}^1\gamma_{i\uparrow}^2 + i\gamma_{i\downarrow}^1\gamma_{i\downarrow}^2)},
$$
 (5)

where  $\phi_i$  represent auxiliary fields living on site i,  $\Delta \tau$  is the imaginary time slice in the Trotter decomposition,  $\lambda = \frac{1}{2} \cosh^{-1}(e^{U\Delta\tau/2})$ , and  $A = \frac{1}{2}e^{-U\Delta\tau/4}$ . It is clear that the decounted Majorana-bilinear operators also respect the decoupled Majorana-bilinear operators also respect both  $T^+ = \sigma^x \tau^z K$  and  $T^- = \sigma^x \tau^z K$  such that this model is sign-problem-free in the Majorana class. We performed projector QMC [10–[12\]](#page-4-18) simulations which show that, with increasing U, the system undergoes a topological quantum phase transition from a topological SC to a trivial SC which breaks time-reversal symmetry spontaneously [\[41\],](#page-4-15) as schematically shown in Fig. [1](#page-3-1). The universality class of this topological phase transition is also obtained by our QMC simulations [\[41\]](#page-4-15).

Concluding remarks.—We have shown that anticommuting MTR symmetries can provide a fundamental principle to identify sign-problem-free interacting models.

<span id="page-3-1"></span>

FIG. 1. The quantum phase diagram of interacting topological superconductors with a topological quantum phase transition as well as the nature of the quantum critical point have been studied by our sign-problem-free QMC simulations [\[41\]](#page-4-15).

Note that this does not contradict the no-go theorem [\[24\],](#page-4-6) as the symmetry principle introduced here may not directly provide recipes of the sign problem for all models. Assuming no other requirement than respecting a set of anticommuting MTR symmetries, we have proved that there are two and only two fundamental sign-problem-free symmetry classes.

Here, we focus on the generic symmetry principle for sign-problem-free models. In the case that the matrices  $h_i$ are not fully random besides respecting the required symmetries, it is possible that sign-problem-free models can be found in the symmetry classes  $\{I\}$ ,  $\{T_1^+\}$ ,  $\{T_1^-\}$ ,  $\{T_1^+\}$ , and  $\{T^+$ ,  $T^+$ ,  $T^+$ ,  $[20, 55]$ . For instance it was  $\{T_1^+, T_2^+\}$ , and  $\{T_1^+, T_2^+, T_3^+\}$  [\[20,55\].](#page-4-19) For instance, it was<br>shown in Refs. [39,55] that certain models in the symmetry shown in Refs. [\[39,55\]](#page-4-14) that certain models in the symmetry class  $\{T_1^+\}$  with special conditions besides the symmetry<br>requirement could be sign-problem-free. In other words it requirement could be sign-problem-free. In other words, it provides hope to avoid the fermion sign problem in various interesting models, such as the repulsive Hubbard model away from half filling [\[12\]](#page-4-20), by utilizing a combination of special features and symmetry principles. We believe that the Majorana-time-reversal symmetry principle has shed new light on avoiding the fermion sign problem in strongly correlated models describing systems such as hightemperature superconductors and featuring exotic quantum critical phenomena [56–[59\].](#page-5-1)

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