

Sign Problem in SSE Monte Carlo for Modified Toric-Code Model

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Toric-Code model is a classical quantum statistic model exhibit topological properties which does not possess the infamous quantum Monte Carlo sign problem. However, certain variants of the Toric-Code model, such as Toric-Code excited states, may encounter a fermionic sign problem. In this study, we employ the Stochastic Series Expansion (SSE) Monte Carlo algorithm to investigate the properties of the Toric-Code model. To address the sign problem, we propose a novel approach that combines basis transformation techniques with the MQMC (Majorana Quantum Monte Carlo) methods.

I. INTRODUCTION

The Toric-Code model [1–4], initially proposed by Alexei Kitaev, is renowned for its remarkable topological properties. With its inherent \mathbf{Z}_2 symmetry, the Toric-Code model stands out as a rare example of a fermionic quantum model that remains unaffected by the infamous fermionic sign problem. Nonetheless, when we perturb the Toric-Code model by modifying its Hamiltonian, such as in the case of Toric-Code excited states, the sign problem reemerges, rendering these modified models non-sign-free.

In this paper, we employ the highly efficient Stochastic Series Expansion (SSE) Monte Carlo algorithm [5, 6] to explore the properties of the Toric-Code model. Furthermore, by introducing additional terms to the Toric-Code Hamiltonian, we intentionally break the intrinsic \mathbf{Z}_2 symmetry, thereby inducing the sign problem in the modified Toric-Code model. To overcome this challenge, we employ the basis transformation method [7] to reconstruct the intrinsic symmetry and successfully eliminate the sign problem in both e and m-excited states of the Toric-Code model.

However, for more complex scenarios such as f-excited states, the traditional basis transformation method proves inadequate. In such cases, we turn to a combined approach, leveraging the SSE Monte Carlo algorithm in conjunction with the Majorana Quantum Monte Carlo (MQMC) method to effectively address the sign problem [8–11].

The rest of this paper is organized as follows: In Section II A, we provide a brief overview of the Toric-Code model, highlighting its key features. In Section II B, we provide a concise review of the Stochastic Series Expansion (SSE) Monte Carlo algorithm, which we employ to study the properties of the Toric-Code model. In Section II C, we delve into the exploration of the Toric-Code model using the SSE Monte Carlo algorithm, analyzing its properties and characteristics. In Section II, we address the sign problem in the Toric-Code model's e and m-excited states through the application of basis transformation techniques, effectively eliminating the sign problem. Building upon the previous section, in Section III, we extend our approach and utilize Majorana

Quantum Monte Carlo (MQMC) methods to tackle the sign problem encountered in the f-excited state of the Toric-Code model. Finally, in Section IV, we conclude the paper by summarizing our findings and discussing their implications.

II. SSE MONTE CARLO FOR TORIC-CODE MODEL

In this section, we explore Toric-Code Model utilizing SSE MC algorithm. Thereafter we would cure sign problem within Toric-Code e and m-excited states via basis transformation method.

A. Toric-Code Model

We begin by briefly reviewing the Toric-Code model [1], which will be explored later through SSE Monte Carlo. Consider a $m \times m$ square lattice on the torus (see fig. 1). Let us attach a spin, or qubit, to each edge of the lattice. (Thus, there are $n = 2m^2$ qubits). For each vertex s and each face p , consider operators of the following form:

$$A_s = \prod_{j \in \text{star}(s)} \sigma_j^x \quad B_p = \prod_{j \in \text{boundary}(p)} \sigma_j^z \quad (1)$$

These operators commute with each other because $\text{star}(s)$ and $\text{boundary}(p)$ have either 0 or 2 common edges. The operators A_s and B_p are Hermitian and have eigenvalues 1 and -1. Now define the Hamiltonian as follows:

$$H_0 = - \sum_s A_s - \sum_p B_p \quad (2)$$

Here, we have defined the Toric-Code model on a torus. Notice that there exists an intrinsic \mathbf{Z}_2 symmetry $A_s \rightarrow B_p$ where the stars s and plaques p are one to one corresponding. Therefore, it is easily proved that Toric-Code model is sign-free in quantum Monte-Carlo.

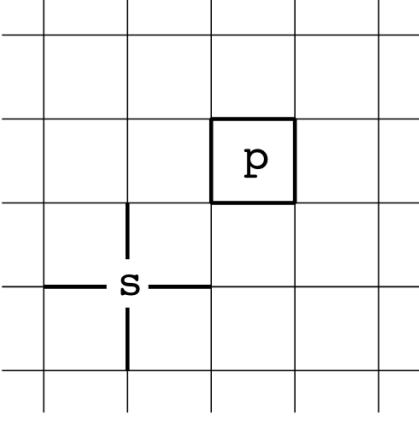


FIG. 1: Toric-Code Model

B. Stochastic Series Expansion QMC Methods

Stochastic series expansion (SSE) algorithm firstly proposed by Anders W. Sandvik [5, 6] is known for its efficiency especially around zero temperature. In this section, we briefly review the SSE method.

Partion function $e^{\beta H}$ is the base for every QMC method, and we start from the Taylor expansion:

$$e^{\beta H} = \sum_{n=0}^{\infty} \frac{-\beta^n}{n!} H^n$$

$$Z = \sum_{n=0}^{\infty} \frac{-\beta^n}{n!} \sum_{\{\alpha\}_n} \langle \alpha_0 | H | \alpha_{n-1} \rangle \dots \langle \alpha_2 | H | \alpha_1 \rangle \langle \alpha_1 | H | \alpha_0 \rangle \quad (3)$$

Very similar to the path integral; For any quantum model, the energy is given as:

$$E = \frac{\langle n \rangle}{\beta} \quad (4)$$

Therefore, we could narrow n-distribution with:

$$\begin{aligned} \langle n \rangle &\propto N\beta \\ \sigma_n &\propto \sqrt{N\beta} \end{aligned} \quad (5)$$

Now, we could fix length scheme by cutting off at $N = L$, fill in with unit operators I :

$$Z = \sum_S \frac{-\beta^n (L-n)!}{L!} \sum_{\{\alpha\}_L} \sum_{\{S_i\}} \langle \alpha_0 | S_L | \alpha_{L-1} \rangle \dots \langle \alpha_1 | S_1 | \alpha_0 \rangle \quad (6)$$

Here n is the number of $S_i = H$ instances in the sequence S_1, \dots, S_L . For a lattice model, we could always write the Hamiltonian as a bond sum of arbitrary lattice:

$$H = -J \sum_{b=1}^{N_b} H_{1,b} + H_{2,b} \quad (7)$$

Here, for a fixed set of basis $H_{1,b}$ represent the diagonal operator, $H_{2,b}$ represent the off-diagonal operator and $H_{0,b} = I$. The partition function for fixed length scheme could be written as:

$$Z = \sum_{\{\alpha\}_L} \sum_{n=0}^L \frac{-\beta^n (L-n)!}{L!} \sum_{\{S_L\}} \langle \alpha | \prod_{p=0}^{L-1} H_{a(p),b(p)} | \alpha \rangle \quad (8)$$

where the index sequence:

$S_L = [a(0), b(0)], [a(1), b(1)], \dots, [a(L-1), b(L-1)]$. With the series expansion above, we could carry out MCMC simulation meanly by the local update and loop update methods see Ref. ? .

C. SSE Monte Carlo For Toric-Code Model

In applying the SSE Monte Carlo method to the Toric-Code model, we initially establish that the conventional SSE loop update algorithm is strictly prohibited in the Toric-Code model (see Appendix for detailed explanation). Consequently, we exclusively employ a combination of local off-diagonal updates and diagonal update processes.

The ground-state phase diagram of the Toric-Code model in the presence of a parallel magnetic field consists of three distinct phases: topological, charge-condensed, and vortex-condensed states (Ref. 4). To investigate the phase transition induced by the parallel field, we introduce modifications to the Hamiltonian as follows:

$$H = H_{toric-code} - h_x \sum_b \sigma_b^x - h_z \sum_b \sigma_b^z \quad (9)$$

The Binder cumulant of μ_s is defined as:

$$Q(\mu_s) = \frac{\langle \mu_s^2 \rangle^2}{\langle \mu_s^4 \rangle} \quad (10)$$

Using our SSE Monte Carlo algorithm and setting $h_x = 0.32$, we analyzed the behavior of the Binder cumulant $Q(\mu_s)$ (refer to Figure 2). The results demonstrate a linear relationship of the Binder cumulant $Q(\mu_s)$ in the vicinity of the critical point, allowing us to determine the critical point at $h_z = 0.335$. Similarly, we found another critical point at $h_z = 0.342$. Notably, the critical points of h_x and h_z approach each other, consistent with the intrinsic \mathbf{Z}_2 symmetry. As a result, we set $h_x = h_z$ and examined the self-duality Binder cumulant (refer to

Figure 3). Our analysis reveals that the first-order transition line initiates around $h_x = h_z = 0.341(2)$, which is in excellent quantitative agreement with the previously reported value of $h_x = h_z = 0.3406$ in Ref. 4.

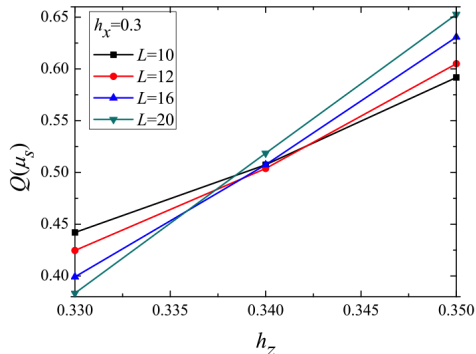


FIG. 2: Binder cumulant $Q(\mu_s)$ for linear system sizes $L = 10, 12, 16, 20$ versus h_z for $h_x = 0.32$.

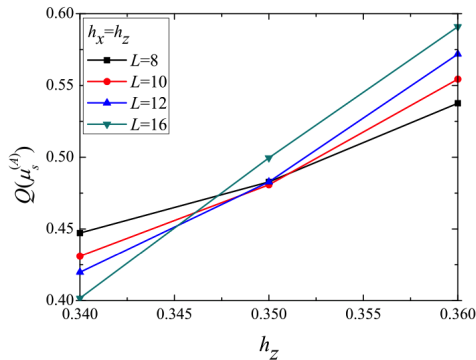


FIG. 3: $Q(\mu_s^A)$ versus h_z along the self-duality line

Furthermore, we present the phase transition diagram of the Toric-Code model in Figure 4. It is noteworthy that, compared to Path integrals Monte Carlo (MC), the SSE Monte Carlo (MC) method exhibits significantly higher efficiency. This enhanced efficiency enables us to simulate system sizes up to 22, which is considerably larger than the 16 achievable with Path integrals MC.

D. Cure Sign Problem in Toric-Code Excited states by Basis Transformation

We induce the sign problem in the modified Toric-Code model by introducing an additional term that breaks the intrinsic \mathbf{Z}_2 symmetry. To transform the Toric-Code Hamiltonian ($H_{\text{toric-code}}$) into the Hamiltonian of the excited states (e, m, f), we can add or subtract specific A_s or B_p terms. However, it is worth noting that the Hamiltonian of the excited states (e, m, f) breaks the

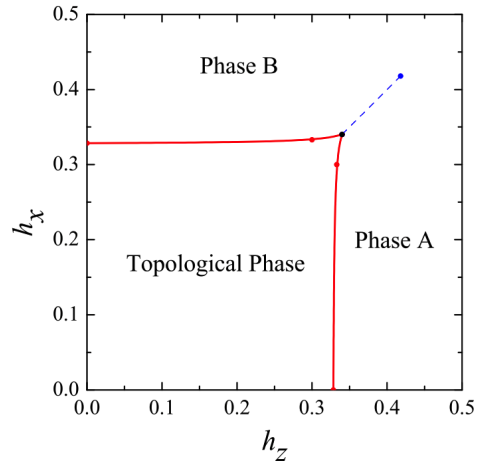


FIG. 4: Phase diagram of the toric code model in magnetic field. The second-order transition lines are shown by full (red) lines and the first-order transition line is represented by dashed (blue) line.

intrinsic \mathbf{Z}_2 symmetry, making them susceptible to the fermionic sign problem.

One conventional approach to address the sign problem involves assigning the absolute value of each weight of the MC process, denoted as $W \rightarrow |W|$, regardless of whether it is negative or complex. However, this method is only applicable when the average sign σ_z approaches unity asymptotically with the inverse temperature β and system size L . Unfortunately, simply implementing this method does not resolve the sign problem of the Toric-Code model within SSE-MC. To tackle this issue, we employ a basis transformation method, as described in Ref. 7. For e-excited states with a positive A_s term in the Hamiltonian, we switch from the eigenstates of the σ_z operator on each site to the eigenstates of the σ_y operators. Conversely, for m-excited states with a positive B_p term in the Hamiltonian, we perform the opposite transformation. This approach effectively transforms the original off-diagonal operators into diagonal operators and vice versa, thereby restoring the intrinsic symmetry.

We then apply the stochastic series expansion (SSE) Monte Carlo simulation for a fixed system size of $L = 16$ to establish the relationship between the inverse temperature β and the average sign $\langle \text{sign} \rangle$ (refer to Figure 5). As the temperature approaches zero, the average sign $\langle \text{sign} \rangle$ tends towards 1, indicating that the influence of the sign problem diminishes as we approach the ground state. Consequently, we can use $|W|$ as a replacement for W to address sign problem within e,m-excited states.

Furthermore, when we fix the temperature to be 1 and vary the size of the system, we observe that as the system size increases, the average sign $\langle \text{sign} \rangle$ also approaches 1 (refer to Figure 6). This indicates that we have addressed the sign problem. However, as we could not transfer the basis to σ_y eigenstates which would result in both A_s and

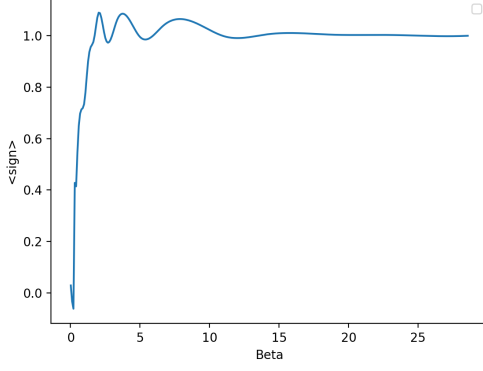


FIG. 5: Average sign $\langle \text{sign} \rangle$ versus inverse temperature β under transformed basis.

B_p to be diagonal, we have to turn another way to cure the sign problem in f-excited state.

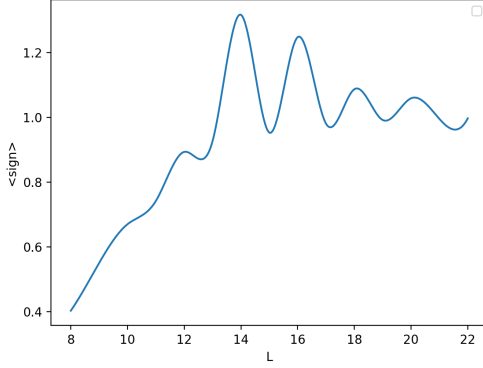


FIG. 6: Average sign $\langle \text{sign} \rangle$ versus system size L under transformed basis.

III. 1D FSPT STATES WITH $G_f = G_b \times_{\omega_2} \mathbb{Z}_2^f$

In this section, we introduce Majorana quantum Monte Carlo (MQMC) method aiming to cure the sign problem within f-excited state of Toric-Code model as well as addressing more generous modified Toric-Code model.

A. Majorana quantum Monte Carlo Method

The Majorana quantum Monte Carlo (MQMC) method is a highly effective technique introduced in Ref. 9 and 10 for solving the fermionic sign problem in interacting fermion models. It utilizes the Majorana representation of complex fermions. MQMC has proven to be particularly successful in tackling the fermionic sign problem in a specific class of models characterized by $SU(N = \text{odd})$ symmetry.

To demonstrate how MQMC can resolve the fermion sign problem in a subset of spinless fermion models, let us consider the following general Hamiltonian for spinless fermions:

$$\begin{aligned} H &= H_0 + H_{int} \\ H_0 &= - \sum_{i,j} [t_{ij} c_i^\dagger c_j + h.c] \\ H_{int} &= \sum_{i,j} V_{ij} (n_i - \frac{1}{2})(n_j - \frac{1}{2}) \end{aligned} \quad (11)$$

The key technique in MQMC method is to rewrite complex fermions operators in Majorana representation:

$$c_i = \frac{1}{2}(\gamma_i^1 + i\gamma_i^2) \quad c_i^\dagger = \frac{1}{2}(\gamma_i^1 - i\gamma_i^2) \quad (12)$$

which enable us to rewrite the Hamiltonian as follows:

$$\begin{aligned} H_0 &= \sum_{i,j} \frac{it}{2} (\gamma_i^1 \gamma_j^1 + \gamma_i^2 \gamma_j^2) \\ H_{int} &= -\frac{V_1}{4} \sum_{\langle i,j \rangle} (\gamma_i^1 \gamma_j^1)(\gamma_i^2 \gamma_j^2) - \frac{V_2}{4} \sum_{\langle\langle i,j \rangle\rangle} (\gamma_i^1 \gamma_j^1)(\gamma_i^2 \gamma_j^2) \end{aligned} \quad (13)$$

In order to ensure symmetry in the two components of Majorana fermions, gauge transformations of the form $c_i \rightarrow ic_i$ are implicitly applied to the Hamiltonian, specifically to the sublattice containing index i . As a result, H_0 can be expressed symmetrically.

Given this context, it becomes evident that in Majorana quantum Monte Carlo (MQMC), Hubbard-Stratonovich (HS) transformations should be performed in the Majorana hopping channels, rather than the density channels as typically done in conventional quantum Monte Carlo (QMC) methods. To be explicit, the HS transformations for the interactions in H_{int} in MQMC are as follows:

$$\begin{aligned} e^{\frac{V_1 \Delta \tau}{4} (i\gamma_i^1 \gamma_j^1)(i\gamma_i^2 \gamma_j^2)} &= \frac{1}{2} \sum_{\sigma_{i,j} = \pm 1} e^{\frac{1}{2} \lambda_1 \sigma_{ij} (i\gamma_i^1 \gamma_j^1 + i\gamma_i^2 \gamma_j^2) - \frac{V_1 \Delta \tau}{4}} \\ e^{\frac{V_2 \Delta \tau}{4} (i\gamma_i^1 \gamma_j^1)(i\gamma_i^2 \gamma_j^2)} &= \frac{1}{2} \sum_{\sigma_{i,j} = \pm 1} e^{\frac{1}{2} \lambda_2 \sigma_{ij} (i\gamma_i^1 \gamma_j^1 - i\gamma_i^2 \gamma_j^2) - \frac{V_2 \Delta \tau}{4}} \end{aligned} \quad (14)$$

The constants λ_1 and λ_2 are determined by the equations $\cosh \lambda_1 = e^{\frac{V_1 \Delta \tau}{2}}$ and $\cosh \lambda_2 = e^{-\frac{V_2 \Delta \tau}{2}}$, respectively. It is important to note that in Eq. (14), the signs of the γ^1 hopping terms are opposite to the γ^2 hopping terms in the Hubbard-Stratonovich (HS) decompositions of the next-nearest-neighbor (NNN) interaction due to the fact that $V_2 < 0$. Similarly, the same signs are obtained for the decoupling of nearest-neighbor (NN) interactions in Eq. (14) because $V_1 > 0$. After the HS transformations,

it becomes apparent that the free fermion Hamiltonian can be split into two parts, each involving only one component of the Majorana fermions. This property ensures that MQMC simulations are free from the sign problem, as the Boltzmann weight becomes positive definite.

IV. CONCLUSIONS

In conclusion, we have investigated the properties of the Toric-Code model and addressed the sign problem that arises when modifying its Hamiltonian. By employing the Stochastic Series Expansion (SSE) Monte Carlo algorithm, we have successfully explored the characteristics of the Toric-Code model. Through the introduction of additional terms to break the intrinsic \mathbf{Z}_2 symmetry, we induced the sign problem in the modified Toric-Code model. However, we were able to overcome this challenge by employing the basis transformation method, which reconstructed the intrinsic symmetry and eliminated the sign problem in both e and m-excited states. For more complex scenarios, such as the f-excited state, the traditional basis transformation method proved inadequate. To address this, we employed a combined approach, leveraging the SSE Monte Carlo algorithm in conjunction with the Majorana Quantum Monte Carlo (MQMC) method. This allowed us to effectively tackle the sign problem encountered in the f-excited state of the Toric-Code model. Our study highlights the importance of understanding and addressing the sign problem in quantum models, particularly when modifying their Hamiltonians. The successful elimination of the sign problem in the Toric-Code model's excited states demonstrates the efficacy of the basis transformation method and the power of the SSE Monte Carlo algorithm in studying these systems. Overall, our findings contribute to the understanding of the Toric-Code model and provide valuable insights into the sign problem in fermionic quantum models. We hope that our work will inspire further research in this field and pave the way for the exploration of other quantum systems with similar sign problems.

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Appendix A: Proof of Prohibition of SSE Loop Update in Toric-Code Model

In this appendix, we rigorously prove that SSE loop update method is strictly forbidden in Toric-Code model. According to Ref. 6, for any given lattice, we have to assign every local site with a bond so as to carry on the update process. And for Toric-Code model the smallest available bond type is shown in figure.7.

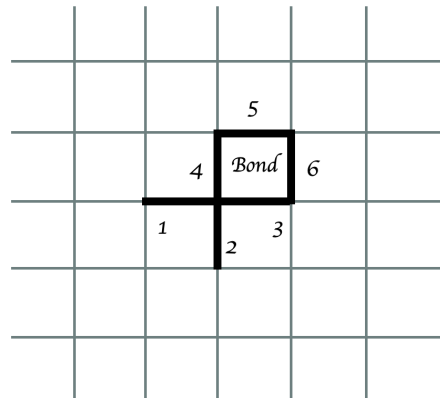


FIG. 7: Bond type of Toric-Code model in SSE Monte Carlo

As B_p is diagonal operator and A_s is off-diagonal operator, it is evident that for a particular bond as shown in figure.7, *side* 1,2,3,4 would change spin direction after the action of off-diagonal operator while *side* 5,6 would not change spin direction because they are only operated by diagonal operator.

To construct a closed loop within the Stochastic Series Expansion Monte Carlo (SSE-MC) process, it is necessary to form a closed path within the Markov chain. In this context, a vertex in the Markov chain corresponds to a specific bond located at site i , with 12 legs representing the spin states before and after the operator acts at that vertex. To create a closed loop, the loop must enter through one leg of the vertex and exit through another leg while simultaneously changing the spin state of both legs. However, it can be easily verified that in order to maintain the vertex as a valid configuration in the Toric-Code model, there must be a simultaneous spin state change of either zero legs or at least four legs. Unfortunately, the loop update process in SSE-MC only allows for a simultaneous spin state change of two legs. As a result, the SSE-MC loop update process is strictly prohibited in the Toric-Code model due to the inability to satisfy the requirements for constructing a closed loop while maintaining the validity of the vertex configurations.

Therefore, other approaches or techniques need to be employed to study the Toric-Code model, taking into account the constraints imposed by the sign problem and the specific characteristics of the model.

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- [1] A. Y. Kitaev, Fault-tolerant quantum computation by anyons, *Annals of Physics* **303**, 2 (2003), arXiv:quant-ph/9707021.
 - [2] M. H. Zarei and A. Montakhab, Phase transition in a noisy Kitaev toric code model [10.48550/ARXIV.1902.06100](#) (2019), publisher: arXiv Version Number: 1.
 - [3] I. S. Tupitsyn, A. Kitaev, N. V. Prokof'ev, and P. C. E. Stamp, Topological multicritical point in the phase diagram of the toric code model and three-dimensional lattice gauge Higgs model, *Physical Review B* **82**, 085114 (2010).
 - [4] J. Vidal, S. Dusuel, and K. P. Schmidt, Low-energy effective theory of the toric code model in a parallel magnetic field, *Physical Review B* **79**, 033109 (2009).
 - [5] R. G. Melko, Stochastic Series Expansion Quantum Monte Carlo, in *Strongly Correlated Systems*, Vol. 176, edited by A. Avella and F. Mancini (Springer Berlin Heidelberg, Berlin, Heidelberg, 2013) pp. 185–206, series Title: Springer Series in Solid-State Sciences.
 - [6] A. W. Sandvik, *Stochastic Series Expansion Methods* (2019), arXiv:1909.10591 [cond-mat].
 - [7] G. Pan and Z. Y. Meng, Sign Problem in Quantum Monte Carlo Simulation (2024) pp. 879–893, arXiv:2204.08777 [cond-mat, physics:hep-lat].
 - [8] E. Berg, M. A. Metlitski, and S. Sachdev, Sign-Problem-Free Quantum Monte Carlo of the Onset of Antiferromagnetism in Metals, *Science* **338**, 1606 (2012).
 - [9] Z.-X. Li, Y.-F. Jiang, and H. Yao, Solving the fermion sign problem in quantum Monte Carlo simulations by Majorana representation, *Physical Review B* **91**, 241117 (2015).
 - [10] Z.-X. Li and H. Yao, Sign-Problem-Free Fermionic Quantum Monte Carlo: Developments and Applications, *Annual Review of Condensed Matter Physics* **10**, 337 (2019).
 - [11] H.-Q. Wu, Y.-Y. He, Y.-Z. You, C. Xu, Z. Y. Meng, and Z.-Y. Lu, Quantum Monte Carlo study of strange correlator in interacting topological insulators, *Physical Review B* **92**, 165123 (2015).