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 multi 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 multi f-excited states 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:

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

These operators commute with each other because star(s) and 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:

$$H_0 = -\sum_s A_s - \sum_p B_p \tag{2}$$

Here, we have defined the Toric-Code model on a torus. Notice that there exists an intrinsic $\mathbf{Z_2}$ symmetry $A_s \to B_p$ where the stars s and plaque p are one to one corresponding. Therefore, it is easily proved that Toric-Code model is sign-free in quantum Monte-Carlo.

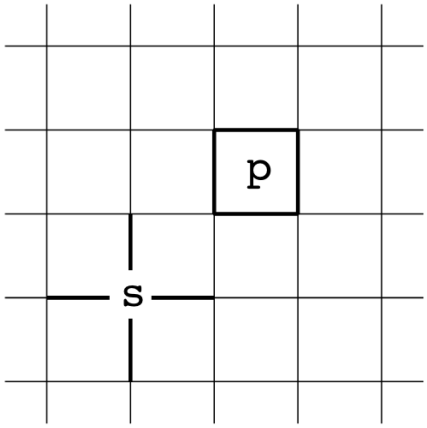

FIG. 1: Toric-Code Model

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:

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

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

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

$$E = \frac{\langle n\rangle}{\beta} \tag{4}$$

Therefore, we could narrow n-distribution with:

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

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

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

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:

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

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:

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

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:

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

The Binder cumulant of μ_s is defined as:

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

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.

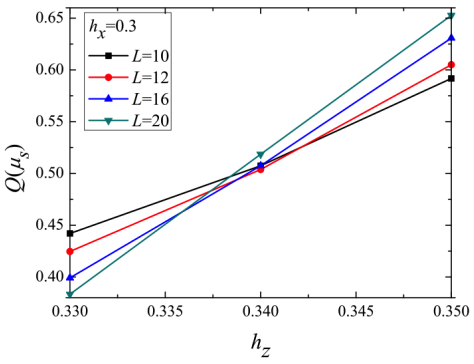

FIG. 2: Binder cumulant $Q(\mu_s)$ for linear sys- tem sizes $L = 10, 12, 16, 20$ versus h_z for $h_x = 0.32$.

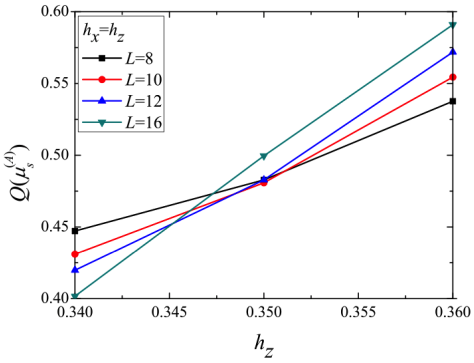

FIG. 3: $Q(\mu_s^A)$ versus h_z along the self-duality line

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) [1], 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 intrinsic $\mathbf{Z_2}$ symmetry, making them susceptible to the fermionic sign problem.

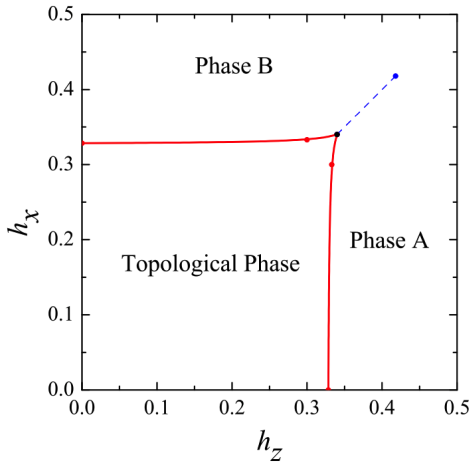

FIG. 4: Phase diagram of the toric code model in magnetic field. The second-order transition lines are shown by full (red) lines and the first-order transition line is repre- sented by dashed (blue) line.

For the e-excited states, we modify the Toric-Code Hamiltonian $H_{\text{toric-code}}$ by adding 2 A_s operators at a particular site s. However, it is easily checked that the e-excited states are immune from the sign problem since A_s is a diagonal operator. It can be deduced that the multi-e-excited states (obtained by adding 2 A_s operators at multiple sites s) are also immune from the fermionic sign problem.

Regarding the m-excited states, we modify the Toric-Code Hamiltonian $H_{\text{toric-code}}$ by adding 2 B_p operators at a particular site p. As B_p is an off-diagonal operator, the sign problem occurs in the m-excited states. However, we can overcome this issue by utilizing a basis transformation method that transforms the basis from the eigenstates of the σ_z operator to those of the σ_x operator. This transformation makes B_p a diagonal operator, effectively resolving the sign problem. The same approach can be generalized to the case of multi-m-excited states.

As for the f-excited states, we modify the Toric-Code Hamiltonian $H_{\text{toric-code}}$ by adding 2 A_s operators at a particular site s and 2 B_p operators at site p. In this case, a simple basis transformation method is not sufficient. One conventional approach to address the sign problem involves assigning the absolute value of each weight of the Monte Carlo process, denoted as $W \to |W|$, 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. To establish the relationship between the inverse temperature β and the average sign $\langle \text{sign} \rangle$, we apply the stochastic series expansion (SSE) Monte Carlo simulation for a fixed system size of $L = 16$ (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 the sign problem within the f-excited states.

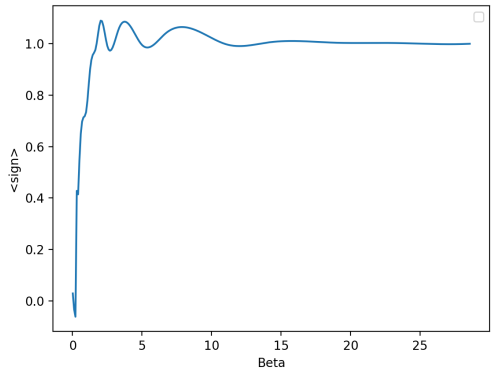

FIG. 5: Average sign $\langle sign \rangle$ versus inverse temperature β under transformed basis.

Furthermore, when we fix the temperature at 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 successfully mitigated the sign problem. However, in situations involving multi f-excited states, the traditional approach of transforming the weight W to its absolute value may not be effective, as the average sign $\langle \text{sign} \rangle$ might not converge to 1 anymore. Therefore, in the next section, we will explore a more systematic method to address the sign problem.

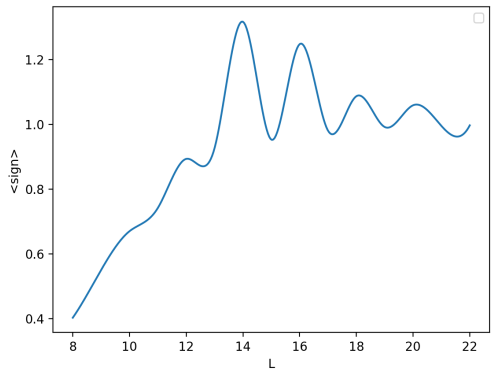

FIG. 6: Average sign $\langle sign \rangle$ versus system size L under transformed basis.

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:

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

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

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

which enable us to rewrite the Hamiltonian as follows:

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

In order to ensure symmetry in the two components of Majorana fermions, gauge transformations of the form $c_i \to i c_i$ 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:

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

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 Toirc-Code Model

In this appendix, we rigorously prove that SSE loop update method is strictly forbbiden 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.

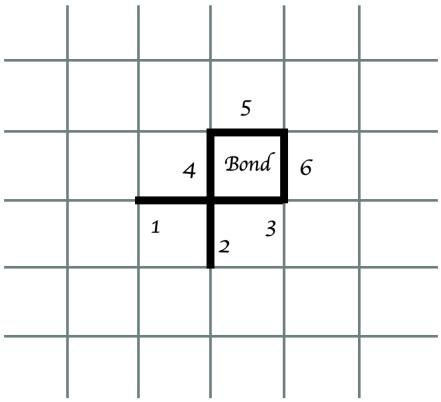

FIG. 7: Bond type of Toric-Code model in SSE Monte Carlo

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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