Stochastic series expansion methods for Heisenberg spin models

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Numerical methods that simulate finite-temperature and ground-state properties of spin models are essential towards the challenge of understanding quantum many-body systems. The stochastic series expansion (SSE) quantum Monte Carlo (QMC) method has been a powerful and efficient numerical approach for discretization-error-free simulation and has been applied to study a large variety of spin systems, the majority of which are $S = 1/2$ Heisenberg models. Here, we review and implement the SSE method in the $S = 1/2$ case. We apply our SSE implementation to estimate the ground state energy of the 1D Heisenberg antiferromagnetic chain to be $\frac{E_{gs}}{N} = -0.443(4)$, in agreement with the exact Bethe ansatz solution, and determine that the leading order finite-size correction to the ground state energy per site scales as N^{-y} for $y = 2(.1)$, consistent with the Luttinger liquid theory of the gapless 1D chain. Additionally, we apply SSE to observe the finite-temperature Néel transition in the Heisenberg antiferromagnet on a cubic lattice. Finally, we discuss the extension of the SSE to $S = 1$ systems, building towards QMC studies of a broader class of quantum systems of both theoretical and experimental interest.

I. INTRODUCTION

The study of quantum many-body physics and statistical physics is closely intertwined, as experimentally observable phenomena in the former arise from interactions between large numbers of microscopic particles, which is well described with the methods and language of the latter. This is well demonstrated by the realm of numerical methods for simulation of quantum many-body physics. A large number of these methods are QMC methods, which revolve around creative methods to sample the exponentially large Hilbert space of an interacting spin system and extrapolate observables to the thermodynamic limit [1, 2].

Here, we provide a review and implementation of the SSE method, which was the first QMC method applied to directly sample the quantum partition function of an interacting spin system beyond the discretized path integral formulation [3], and apply it to study low-temperature behavior and finite-temperature phase transitions for the spin-1/2 Heisenberg antiferromagnet in 1D and 3D respectively. We then discuss the extension of the SSE method to spin-1 systems. Despite being less explored than the spin-1/2 case with SSE algorithms, spin-1 many-body systems host a broad range of interesting new physics, such as the gapped Haldane chain [4], spin-nematic phases [5], and novel quantum critical behavior absent in spin-1/2 [6]. We proceed to describe the general SSE philosophy here and specific implementation for $S = 1/2$ Heisenberg spin models in Sec. II, and describe results of SSE QMC study of 1D and 3D $S = 1/2$ Heisenberg antiferromagnets in Sec. III. We describe a possible extension to $S = 1$ in Sec. IV and conclude in Sec. V.

We follow the treatment in Ref. [3] to introduce the SSE QMC method in the $S = 1/2$ setting, which was introduced and developed in Refs. [7, 8]; as its name suggests, the SSE QMC algorithm estimates the partition function $Z = \mathrm{tr}\{e^{-\beta\mathcal{H}}\}$ through Monte Carlo sampling of terms in the series expansion

$$\mathrm{Tr}\exp(-\beta\mathcal{H}) = \sum_{\{s_i\}_0} \langle\{s_i\}_0| \left(\sum_{n=0}^{\infty} \frac{1}{n!}(-\beta\mathcal{H})^n\right) |\{s_i\}_0\rangle \tag{1}$$

where the outer sum ranges over a basis for all many-body states in a system of N particles. For simplicity, we consider the basis of all product states given a local basis for the one-particle Hilbert space, which we denote $|\{s_i\}\rangle \equiv |s_1\rangle \otimes |s_2\rangle \otimes \cdots \otimes |s_N\rangle$, where each s_i represents the local state of particle i.

The indexing of $\{s_i\}_0$ in Eqn. 1 foreshadows the introduction of additional copies of the product state basis in computing Z. Indeed, as the many-body identity operator $I = \sum_{\{s_i\}} |\{s_i\}\rangle \langle\{s_i\}|$, we have

$$\mathrm{Tr}\exp(-\beta\mathcal{H}) = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{s_i\}_0,\{s_i\}_1,\ldots,\{s_i\}_{n-1}} \left(\prod_{j=0}^{n-1} \langle\{s_i\}_j| \mathcal{H} \left|\{s_i\}_{j+1 \pmod n}\right\rangle\right) \tag{2}$$

Therefore, for a Hamiltonian $\mathcal{H}$ describing the physics of nearest-neighbor interactions through local bond operators $B(s_a, s_b)$ that act only the two-particle Hilbert space of nearest-neighbors a and b,

$$\mathcal{H} = \sum_{\langle a,b\rangle} \sum_{c} B_c(s_a, s_b) \tag{3}$$

where c indexes perhaps different modes of interaction (onsite, direct exchange, antisymmetric exchange, etc.), the term in Z associated with the product state configuration $\{s_i\}_0, \{s_i\}_1, \ldots, \{s_i\}_{n-1}$ is nonzero only if for each $\{s_i\}_j$ in the configuration, there exists some a, b, c such that $\langle s_{a,j+1}, s_{b,j+1}| B_c(s_a, s_b) |s_{a,j+1}, s_{b,j+1}\rangle \neq 0$.

Through the use of local bond operators $B_{c_j}(s_{a_j}, s_{b_j})$, we can re-define each $\{s_i\}_j$ recursively through

$$|\{s_i\}_{j+1}\rangle \equiv B_{c_j}(s_{a_j}, s_{b_j})\,|\{s_i\}_j\rangle \tag{4}$$

where changes from $|\{s_i\}_j\rangle$ to $|\{s_i\}_{j+1}\rangle$ can only occur locally at bond $\langle a_j, b_j\rangle$. Thus, each term in Z is uniquely defined by the starting configuration $\{s_i\}_0$ and the utilized bond operators $B_{c_0}(s_{a_0}, s_{b_0}), \ldots, B_{c_{n-1}}(s_{a_{n-1}}, s_{b_{n-1}})$; therefore, we can simplify Eqn. 2:

$$\begin{aligned}\mathrm{Tr}\exp(-\beta\mathcal{H}) = \sum_{n=0}^{\infty}\frac{(-\beta)^n}{n!} \\ \sum_{\{s_i\}_0}\sum_{B_{c_0}(s_{a_0},s_{b_0}),\ldots,B_{c_{n-1}}(s_{a_{n-1}},s_{b_{n-1}})} \\ \left(\prod_{j=0}^{n-1}\langle\{s_i\}_j|\,B_{c_j}(s_{a_j},s_{b_j})\,|\{s_i\}_{j+1 \pmod n}\rangle\right)\end{aligned} \tag{5}$$

The SSE constructs a Markov chain between states S parameterized by n, $\{s_i\}_0$, and $(a_0, b_0, c_0), (a_1, b_1, c_1), \ldots, (a_{n-1}, b_{n-1}, c_{n-1})$, with associated weight $W(S)$ where

$$\begin{aligned}W(S) &= \frac{(-\beta)^n}{n!}\prod_{j=0}^{n-1}\langle\{s_i\}_j|\,B_{c_j}(s_{a_j},s_{b_j})\,|\{s_i\}_{j+1 \pmod n}\rangle \\ &= \frac{\beta^n}{n!}\prod_{j=0}^{n-1}\langle\{s_i\}_j|-B_{c_j}(s_{a_j},s_{b_j})\,|\{s_i\}_{j+1 \pmod n}\rangle\end{aligned} \tag{6}$$

is the contribution of state S to Z according to Eqn. 5. We use a scheme such as Metropolis-Hastings, where detailed balance is satisfied, ie. for a state S, an update to state S' is proposed; then, it is accepted with probability

$$p_{\text{accept}} = \min(1, \frac{W(S')}{W(S)}\cdot\frac{p_{\text{propose}}(S\to S')}{p_{\text{propose}}(S'\to S)}) \tag{7}$$

We note that $W(S)$ is not *a priori* guaranteed to be positive, and indeed breaks this requirement for well-definedness of p_{accept} for many spin-models of interest, which is a well-known manifestation of the QMC sign problem. In this paper, we concern ourselves with the physics of sign-problem-free models. In applying the SSE to a specific spin model with N sites and defined nearest neighbor connections $\langle a, b\rangle$, it is necessary to define a local basis at each site to populate $\{s\}$ as well the allowed nearest-neighbor interactions B between sites, which are essential to defining a state in the Markov chain and properly avoid the sign problem. Then, we define the method to propose updates from state S to another state S' and calculating the transition probability for the update efficiently. The effectiveness and efficiency of this step is critical in the performance of the QMC algorithm: if S' is generically too similar to S, then the algorithm will not ergodically sample the state space within a reasonable number of Monte Carlo steps; on the other hand, if S' is generically too different from S, then the recalculation of $\frac{W(S')}{W(S)}$ after each proposed step would be prohibitively expensive computationally.

II. THE SPIN-1/2 HEISENBERG ANTIFERROMAGNET

In the spin-1/2 case, we choose the local basis to be the $\hat{S}_z$ eigenbasis for some arbitrarily chosen preferred axis z and denote states $|\pm\rangle$ such that $\hat{S}_z\,|\pm\rangle = \pm\frac{1}{2}\,|\pm\rangle$. We consider the Heisenberg Hamiltonian

$$\mathcal{H} = J\sum_{\langle a,b\rangle}\mathbf{S}^a\cdot\mathbf{S}^b = J\sum_{\langle a,b\rangle}S_z^aS_z^b + \frac{1}{2}(S_+^aS_-^b + S_-^aS_+^b) \tag{8}$$

for an antiferromagnet ($J > 0$). We note that as Eqn. 8 is easily decomposed to operators that act purely diagonally and off-diagonally in the $|\pm\rangle\otimes|\pm\rangle$ basis, which foreshadows our definition of the B_c operators. First, the diagonal term in this basis is

$$-S_z^aS_z^b = \begin{pmatrix}-1/4 & 0 & 0 & 0\\ 0 & 1/4 & 0 & 0\\ 0 & 0 & 1/4 & 0\\ 0 & 0 & 0 & -1/4\end{pmatrix} \tag{9}$$

To avoid the sign problem, we instead take the diagonal operator ($c = 1$) to be $-B_1 = \frac{1}{4}I_4 - S_z^aS_z^b$ such that the only nonzero matrix elements are $\langle+-|-B_1\,|+-\rangle = \langle-+|-B_1\,|-+\rangle = +1/2$; note that this corresponds to adding a global term to the many-body Hamiltonian $\mathcal{H}$ of $\frac{N_b}{4}I$ which has a trivial effect on its spectrum. The off-diagonal operator is

$$-B_2 = -\frac{1}{2}(S_+^aS_-^b + S_-^aS_+^b) = \begin{pmatrix}0 & 0 & 0 & 0\\ 0 & 0 & -1/2 & 0\\ 0 & -1/2 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix} \tag{10}$$

We note that for any state S, $W(S)$ is nonzero only if

$$\begin{aligned}|\{s_i\}_0\rangle &= B_{c_{n-1}}(s_{a_{n-1}}, s_{b_{n-1}})\,|\{s_i\}_{n-1}\rangle \\ &= \left(\prod_{j=0}^{n-1}B_{c_j}(s_{a_j},s_{b_j})\right)|\{s_i\}_0\rangle\end{aligned} \tag{11}$$

If the lattice is bipartite, it is required that an even number of off-diagonal operators are required to take any site a back to itself. Therefore, the contribution of off-diagonal operators to $W(S)$ appears as $(-1/2)^M > 0$ for even M, so the choice of $-B_2 = -\frac{1}{2}(S_+^aS_-^b + S_-^aS_+^b)$ is sign-problem-free on a bipartite lattice.

Given the bipartite lattice with N sites and N_b bonds connecting nearest neighbor sites, the QMC algorithm can be initialized via a random selection of $\{s_i\}_0 = |\pm\rangle^{\otimes N}$ and $n = 0$ with no operators. For computational

purposes, we introduce the maximum expansion order $L > n$ and set it to some fiducial starting value, along with a dummy operator $-B_0 = I_4$. For any Monte Carlo step, there will be $L - n$ instances of the B_0 operator, which exist in order to guarantee that n will never exceed our cap L; in the extreme case of the initial step, all operators are set to B_0.

The Monte Carlo update process proceeds in two steps. First, the "diagonal update" iterates from $l = 1, \ldots, L$. If the operator is B_0, we select an edge $\langle a_l, b_l \rangle$ over all edges uniformly at random and propose the update $B_0 \to B_1(a_l, b_l)$ if $|a_l b_l\rangle = |{+}{-}\rangle$ or $|a_l b_l\rangle = |{-}{+}\rangle$ (ie. the two basis elements with nonzero B_1 matrix element). Instead, if the operator is $B_1(a_l, b_l)$ for some $\langle a_l, b_l \rangle$, we propose the opposite update $B_1(a_l, b_l) \to B_0$. Per Eqn. 7, we have that for the forward update, $\frac{W(S')}{W(S)} = \frac{\beta}{2}$ and $\frac{p_{\text{propose}}(S \to S')}{p_{\text{propose}}(S' \to S)} = \frac{N_b}{L-n}$ [1], so the total

$$p_{\text{accept}} = \frac{N_b \beta / 2}{L - n} \tag{12}$$

Similarly, the reverse update occurs with probability

$$p_{\text{accept}} = \frac{L - n + 1}{N_b \beta / 2} \tag{13}$$

Finally, if $L - n$ becomes small due to the introduction of new diagonal operators, L is incremented (e.g. to $1.1L$) and the new operators are initialized to B_0.

Second, the "off-diagonal update" occurs by constructing an operator loop, an approach which was first-introduced in Ref. [9]. The operator loop is constructed by randomly selecting some site $a_0 \in 1, \ldots, N$ and some expansion order $l_0 \in 1, \ldots, L$, then performing a walk in (a, l) space according the following algorithm: increase l_0 until encountering an edge $\langle a_0, b_0 \rangle$ for some other site b_0 such that $B_c(a_0, b_0)$ has $c = 1$ or $c = 2$, potentially crossing through $l = 0$. Then, hop from site a_0 to b_0 and change direction in l. This algorithm continues until returning to (a_0, l_0), which is guaranteed per Eqn. 11. Then, we propose the update of switching all encountered operators $B_c(a, b)$ from $c = 1 \leftrightarrow 2$ and $s_{a_0} \to -s_{a_0}$ for all sites a for which the loop crossed through $l = 0$. Since all matrix elements of both B_1 and B_2 have magnitude $\frac{1}{2}$ and biparticity guarantees the absence of the sign problem, $\frac{W(S')}{W(S)} = 1$. Similarly, $\frac{p_{\text{propose}}(S \to S')}{p_{\text{propose}}(S' \to S)} = 1$ as the loop construction is agnostic towards if any operator B is of the diagonal or off-diagonal type. Therefore, the off-diagonal update is always accepted. Because of the triviality of calculating this transition probability involved in performing a global operator-loop update that can change many operators, it addresses both qualitative criteria for an effective QMC sampling scheme described in Sec. I. Thus, it was seen as a breakthrough for practical SSE calculation.

[1] There are N_b bonds possible to select to insert B_1, but the reverse update has only one pathway possible to remove B_1 existing at a pre-determined edge. The factor of $L - n$ in the denominator reflects that there are $\binom{L}{L-n}$ ways to allocate the identity elements B_0 among $l = 1, \ldots, L$, but all ways are physically equivalent to a single term in Z. Upon addition of a diagonal operator B_1, this number decreases to $\binom{L}{L-n-1}$

III. RESULTS

For the term project, I implemented the SSE QMC algorithm for the spin-1/2 Heisenberg magnet in Julia. I used the method to study the ground state energy of a one-dimensional antiferromagnetic spin chain and critical behavior near the finite-temperature Néel transition in the three-dimensional Heisenberg antiferromagnet. We discuss both settings below.

A. Ground state energy of the $S = 1/2$ Heisenberg AFM chain

To validate our implementation and calibrate performance, we first apply the SSE method to the spin-1/2 antiferromagnetic Heisenberg chain, a canonical model with an exactly known ground state energy in the thermodynamic limit of $N(-\ln 2 + 1/4) \approx -0.443147N$ from the exact Bethe ansatz solution [10]. This model captures essential features of quantum strong correlation in one dimension and is thus both a benchmark of SSE performance as well as a setting to study finite-size scaling of ground state properties.

The ground state energy is estimated from SSE QMC as follows; as

$$\langle E \rangle = -\frac{\partial Z}{\partial \beta} \tag{14}$$

direct evaluation from Eqn. 5 gives

$$\begin{aligned}
\langle E \rangle &= -\sum_{n=0}^{\infty} n(-1)^n \frac{(\beta)^{n-1}}{n!} \sum_{\{s_i\}_0} \sum_{B_{c_0}(s_{a_0}, s_{b_0}), \ldots, B_{c_{n-1}}(s_{a_{n-1}}, s_{b_{n-1}})} \\
&\quad \left(\prod_{j=0}^{n-1} \langle \{s_i\}_j | \, B_{c_j}(s_{a_j}, s_{b_j}) \, | \{s_i\}_{j+1 \pmod n} \rangle \right) \\
&= -\sum_{n=0}^{\infty} \frac{n}{\beta} \frac{(-\beta)^n}{n!} \sum_{\{s_i\}_0} \sum_{B_{c_0}(s_{a_0}, s_{b_0}), \ldots, B_{c_{n-1}}(s_{a_{n-1}}, s_{b_{n-1}})} \\
&\quad \left(\prod_{j=0}^{n-1} \langle \{s_i\}_j | \, B_{c_j}(s_{a_j}, s_{b_j}) \, | \{s_i\}_{j+1 \pmod n} \rangle \right) = -\frac{\langle n \rangle}{\beta}
\end{aligned} \tag{15}$$

Thus, storing the value of n at each Monte Carlo step for a simulation at fixed β allows for calculation of $\langle E \rangle$. We perform such a calculation at $N = 4, 8, 12, 16, 20, 24$ for $\beta =$

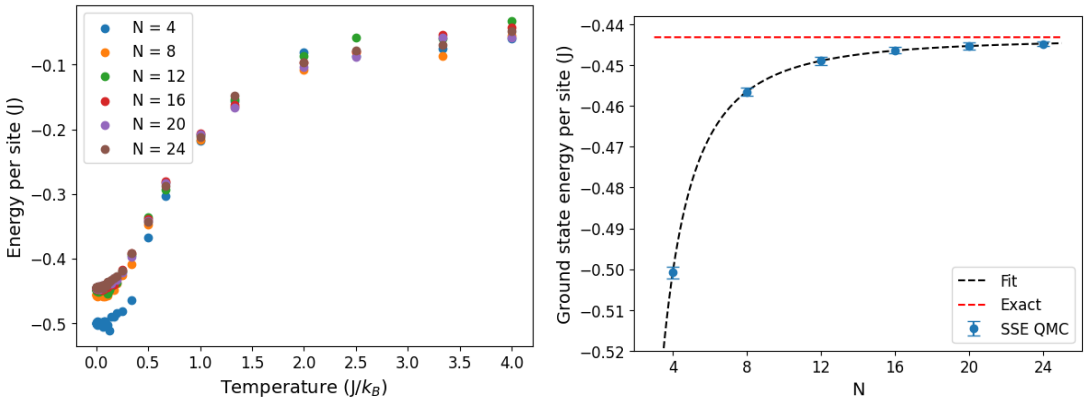

Fig. 1: (L) SSE QMC predicted values for $\langle E \rangle$ of the 1D Heisenberg $S = 1/2$ antiferromagnetic chain at finite temperature. (R) Extrapolation of $\langle E \rangle$ to the $\beta, N \to \infty$ limit provides excellent agreement with the exact Bethe ansatz energy for the 1D $S = 1/2$ Heisenberg antiferromagnetic chain.

$0.25, 0.3, 0.4, 0.5, 0.75, 1, 1.5, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 14, 16, 18, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 600, 700, 800$ and perform 5000 Monte Carlo steps for each (β, N), discarding the first 1000 steps for startup transience (Fig. 1(L)). For each N, we then extrapolate the calculated $\frac{\langle E \rangle}{N}$ to $T \to 0$ and fit the resulting ground state energy to the functional form (Fig.. 1(R)).

$$\frac{E(N)}{N} = E_{gs} + cN^{-y} \tag{16}$$

We find that $\frac{E_{gs}}{N} = -0.443(4)$, in excellent agreement with the energy predicted by the exact Bethe ansatz solution. Furthermore, we find that the leading low-temperature finite-size correction is given by the exponent $y = 2(.1)$, consistent with the exact exponent of 2 given by the universality class of gapless 1D systems described by the Luttinger liquid theory [11].

B. Finite temperature phase transition in three dimensions

Next, we examine the finite-temperature phase transition of the three-dimensional (3D) spin-1/2 Heisenberg antiferromagnet on the cubic lattice. At a finite critical temperature T_c, the system undergoes a continuous transition from a paramagnetic to a Néel-ordered phase, characterized by spontaneous breaking of SU(2) spin rotation symmetry. We calculate the finite-temperature heat capacity as a function of β similarly by taking another derivative with respect to β of Eqn. 15 to find that

$$C = \langle n^2 \rangle - \langle n \rangle^2 - \langle n \rangle \tag{17}$$

We perform SSE QMC of the $S = 1/2$ Heisenberg antiferromagnet on the $N =$ 5x5x5 cubic lattice and plot the heat capacity in Fig. 2. We find results consistent with the reported numerically calculated transition temperature of $\frac{T_c}{J} = 0.946$ when extrapolated to $N \to \infty$ [12].

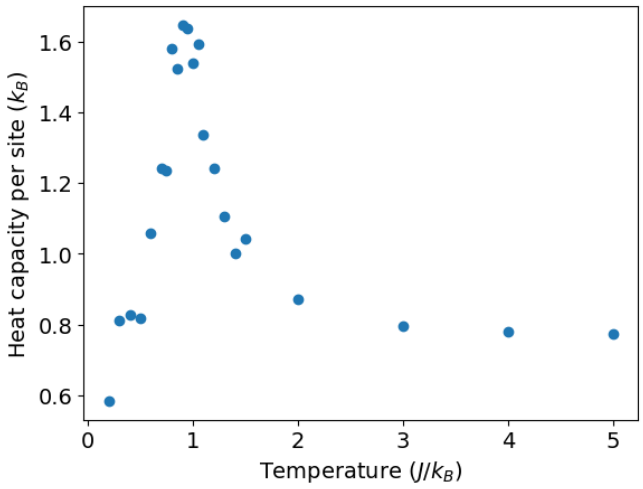

Fig. 2: Finite-temperature heat capacity of the $S = 1/2$ Heisenberg antiferromagnet on the cubic lattice. The peak in heat capacity below $\frac{T}{J} = 1$ is consistent with the Néel transition, with a flat-topped cusp consistent with slightly negative critical exponent α.

Furthermore, the cusp in the heat capacity is consistent with the negative critical exponent $\alpha = -0.1336(15)$ [13] for

$$\ln Z \propto T^{2-\alpha} \tag{18}$$

However, SSE QMC results near T_c were sufficiently noisy due to large scale-invariant fluctuations to ensure accurate fitting of such critical exponent difficult.

IV. EXTENSION TO SPIN-1

While our results have primarily focused on the spin-1/2 case, the additional physics in spin-1 systems is also

amenable to SSE calculation. The expanded local $\hat{S}^z$ eigenbasis of $|1\rangle, |0\rangle, |-1\rangle$ leads to new quantitative behaviors, which is particularly evident through the generic spin-1 Hamiltonian

$$\mathcal{H} = \sum_{\langle a,b\rangle} J\mathbf{S}^a \cdot \mathbf{S}^b + K(\mathbf{S}^a \cdot \mathbf{S}^b)^2 + \sum_a D(\mathbf{S}^a_z)^2 \tag{19}$$

with biquadratic and single-ion anisotropy terms indexed by K and D respectively that are trivial in the spin-1/2 case. Below, we consider the specific SSE extension that occurs for $D \neq 0$, $K = 0$, which in addition to the Néel and disordered phases, supports a quantum phase transition to a $|0\rangle$ dominated phase at large D, as well as exotic periodic combinations of such orderings [14]. Although there are some implementations and results of SSE QMC in $S = 1$ [15, 16], the vast majority of existing SSE QMC literature and other notes and discussion [3, 17] focus exclusively on $S = 1/2$. Here, we discuss the challenges and solutions from extending the previous approach to $S = 1$.

Following the principles outlined in Secs. I and II, we define the corresponding operators and spin states involved for the spin-1 Hamiltonian in order to define the corresponding Markov chain on states parameterized by the ordered product of local bond operators on an initial product state to estimate the many-body partition function. We then describe the extension of diagonal and off-diagonal updates to propose updates in the state space. Here, bond operators act on a 9-dimensional Hilbert space, which we again use the basis given by the pairwise tensor product of $(|1\rangle, |0\rangle, |-1\rangle)$. Rewriting

$$\sum_{\langle a,b\rangle} J\mathbf{S}^a \cdot \mathbf{S}^b + \sum_a D(\mathbf{S}^a_z)^2 = \sum_{\langle a,b\rangle} S^a_z S^b_z + \frac{D}{z}\left((\mathbf{S}^a_z)^2 + (\mathbf{S}^b_z)^2\right) + \frac{1}{2}(S^a_+ S^b_- + S^a_- S^b_+) \tag{20}$$

assuming that each site has z nearest neighbors in the lattice, we see that the local anisotropy term can be absorbed in the diagonal operator. The diagonal matrix elements of $\mathcal{H}$ are thus

$$\begin{aligned} - S^a_z S^b_z - \frac{D}{z}\left((\mathbf{S}^a_z)^2 + (\mathbf{S}^b_z)^2\right) = \\ \mathrm{diag}(-1 - \frac{2D}{z}, -\frac{D}{z}, +1 - \frac{2D}{z}, \\ -\frac{D}{z}, 0, -\frac{D}{z}, \\ +1 - \frac{2D}{z}, -\frac{D}{z}, -1 - \frac{2D}{z}) \end{aligned} \tag{21}$$

Similarly to the spin-1/2, we then let the diagonal operator $-B_1 = -S^a_z S^b_z - \frac{D}{z}\left((\mathbf{S}^a_z)^2 + (\mathbf{S}^b_z)^2\right) + (1 + \frac{2D}{z})I$ to ensure positivity in the $D > 0$ case. Calculating the off-diagonal operator analogously gives

$$-B_2 = -\frac{1}{2}(S^a_+ S^b_- + S^a_- S^b_+) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{22}$$

Again, for bipartite lattices, this choice of B_2 ensures sign-problem-free QMC. However, two significant qualitative differences in B_1 and B_2 lead to qualitatively different implementations of Monte Carlo transition proposals and probabilites relative to the $S = 1/2$ case. First, the $S = 1/2$ case was convenient in that all matrix elements of both B_1 and B_2 had magnitude $\frac{1}{2}$; here, the introduction of $D > 0$ leads to distinct bond operator matrix elements. This can be compensated for in the diagonal update through modifying the transition probability in Eqn. 12 to

$$p_{\text{accept}} = \frac{N_b \beta \langle s_a s_b| - B_1 |s_a s_b\rangle}{L - n} \tag{23}$$

for introducing a diagonal operator and analogously for destroying a diagonal operator for bond $\langle a, b\rangle$ chosen uniformly at random. Furthermore, as these matrix elements are distinct from those of B_2, the probability for accepting a proposed loop update also differ from 1; in a practical implementation, this can be calculated in parallel to loop traversal through incurring a rolling product of

$$\left(\frac{1}{\langle s_a s_b| - B_1 |s_a s_b\rangle}\right)^{\pm 1} \tag{24}$$

for each encountered bond $\langle a, b\rangle$, for exponent $+1$ for a diagonal to off-diagonal update and -1 for the opposite case, as all B_2 matrix elements have magnitude 1.

Second, the off-diagonal operator is no longer closed, as $B_2 |00\rangle = |+1 - 1\rangle + |-1 + 1\rangle$. As such, for a given encountered off-diagonal operator acting on state $|00\rangle$, an arbitrary choice must be made with regards to consider the $|+1 - 1\rangle$ branch or $|-1 + 1\rangle$ branch. Such choice incurs an additional factor of $\frac{1}{2}$ on the transition probability due to the proposal probability ratio term in Eqn. 7, and 2 for the inverted setting. However, such an "incorrect" arbitrary choice can break closure of the loop, such that $\{s_i\}_{L-1}$ is no longer connected via bond operator to $\{s_i\}_0$; in such a scenario, the update accept probability defaults to 0. As a result, such a Markov chain inherent explores the state space at a slower rate. Instead, alternative loop construction algorithms have been developed to avoid such decisions for global off-diagonal updates, such as that presented in full in Ref. [15].

V. CONCLUSIONS

In this paper, we studied the SSE QMC method through implementation for two well-understood quantum spin-1/2 systems: the 1D Heisenberg antiferromagnetic chain and the finite-temperature Néel transition on a cubic lattice. Our results reproduce exact and known values. Building on this foundation, we discussed methods for extending SSE to spin-1 quantum magnets. These systems exhibit richer physics of ground states and quantum phase transitions due to their enlarged local Hilbert space and new interactions. As future work, I hope to implement such methods to study spin-1 physics with bilinear-biquadratic interactions and local anisotropy to explore quantum phases of interacting spin-1 moments new lattices, especially those realized in new condensed matter or atomic physics experiments.

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