Resummation-based quantum Monte Carlo vis-à-vis sign-problematic $S = \frac{1}{2}$ Heisenberg models on canonical geometrically frustrated lattices

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Abstract. We show here that a direct application of resummation-based quantum Monte Carlo (QMC) — implemented recently for sign-problem-free $SU(2)$-symmetric spin Hamiltonians in the stochastic series expansion (SSE) framework — does not reduce the sign problem for frustrated $SU(2)$-symmetric $S = \frac{1}{2}$ Heisenberg antiferromagnets on canonical geometrically frustrated lattices composed of triangular motifs such as the triangular lattice. In the process, we demonstrate that resummation-based updates do provide an ergodic sampling of the SSE-based QMC configurations which can be an issue when using the standard SSE updates, however, severely limited by the sign problem as previously mentioned. The notions laid out in these notes may be useful in the design of better algorithms for geometrically frustrated magnets.

Keywords. Quantum Monte Carlo; stochastic series expansion; resummation-based updates; Heisenberg models.

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1. Introduction

We give an outline of this brief report. In Section 2, we set the stage by briefly recapitulating the standard SSE set-up and resummation-based updates as they apply to sign-problem-free $S = \frac{1}{2}$ Hamiltonians on geometrically unfrustrated, bipartite lattices. Here, we also give a reason for why one might expect resummation to lead to a possible reduction in the sign problem for geometrically frustrated, non-bipartite lattices. In Section 3, we build towards describing which kind of SSE-based QMC configurations, if they were to exist, would lead to a reduction of the sign problem with resummation. We then give an argument for why such configurations do not exist for $S = \frac{1}{2}$ Heisenberg antiferromagnets on canonical geometrically frustrated lattices made out of triangular motifs. Section 3 also discusses how resummation-based updates allow for an ergodic sampling of the sign-problematic frustrated QMC ensemble (limited by the sign problem) and a closely related sign-problem-free ensemble.

2. SSE basics

The SSE framework and SSE-based QMC has been extensively discussed in the literature. For a detailed exposition, the reader may see the following reviews [1, 2]. Here we limit ourselves to the basic notions underlying the SSE framework that are required for the subsequent sign problem discussions in Section 3. The equilibrium statistical physics of a quantum Hamiltonian $H$ is studied by computing the quantum partition function

$$Z = \text{Tr}(e^{-\beta H}).$$

In SSE, the quantum to classical mapping is carried out by expanding this exponential in a Taylor series. After writing the trace as an expansion in a chosen basis, the partition function is expressed as follows:

$$Z = \sum_{\alpha} \langle \alpha | e^{-\beta H} | \alpha \rangle = \sum_{\alpha} \langle \alpha | \sum_{n} \frac{(-\beta H)^n}{n!} | \alpha \rangle,$$
where \(|\{\alpha\}\rangle\) is the chosen basis. If we introduce a complete set of states between each power of \(H\), this series can be written as
\[
Z = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_{\{\alpha\}_n} \langle \alpha_0 | (-H) | \alpha_1 \rangle \cdots \langle \alpha_{n-1} | (-H) | \alpha_0 \rangle. \tag{3}
\]
The \(|\{\alpha\}_n\rangle\) indicates there are \(n\) states to sum over. This brings it into a form where each term in the sum consists of a sequence of spin states: \(|\alpha_0\rangle, |\alpha_1\rangle, |\alpha_2\rangle \cdots |\alpha_{n-1}\rangle, |\alpha_0\rangle\) for a given \(n\). The subscript \(i = 0, 1, \ldots, n - 1\) in \(\alpha_i\) can be related to the “imaginary time” dimension and hence a particular sequence of spin states \(|\{\alpha\}_n\rangle\) can be interpreted as a classical spin configuration in one extra dimension. The different sequences of \(|\{\alpha\}_n\rangle\) are sampled stochastically with their corresponding weight, \(W(|\{\alpha\}_n\rangle, \beta)\). This weight is proportional to the product of all the matrix elements in eq. (3) evaluated in this sequence as follows:
\[
W(|\{\alpha\}_n\rangle, \beta) = \frac{\beta^n}{n!} \prod_{i=0}^{n-1} \langle \alpha_i | (-H) | \alpha_{i+1} \rangle, \tag{4}
\]
where we necessarily have \(|\alpha_n\rangle = |\alpha_0\rangle\) due to the trace operation in the partition function (“periodic boundary condition in imaginary time dimension”). For an arbitrary \(H\), however, every term in the series in eq. (3) need not have a positive weight resulting in the notorious sign problem. For a Hamiltonian to be amenable to QMC simulations, a sufficient condition is the following:
\[
\langle \alpha_i | H | \alpha_j \rangle \leq 0, \quad \forall \ i, j. \tag{5}
\]
The diagonal matrix elements can be made negative by subtracting a large constant, therefore the above condition really concerns the off-diagonal matrix elements when designing or discussing algorithms. This condition is equivalent to what is sometimes also referred to as the Marshall sign rule. The Heisenberg antiferromagnet on a bipartite lattice, is an example of a sign-problem-free model, where these classical configurations can be further interpreted as closely-packed loop configurations.

2.1 The Heisenberg antiferromagnet as an example

The Heisenberg interaction between two sites \(i\) and \(j\), up to a constant \(S^2\), can be written as
\[
H^{ij}_2 = -J (S_i^z - \vec{S}_i \cdot \vec{S}_j), \tag{6}
\]
where \(S\) is the value of the spin. The subtraction of \(S^2\) makes all diagonal elements negative and a unitary transformation on one of the sites (say \(S_j^z \rightarrow -S_j^z\) and \(S_j^y \rightarrow -S_j^y\)) makes all the off-diagonal elements of \(H^{ij}_2\) negative satisfying the condition in eq. (5). By carrying out this unitary transformation on one of the sublattices of the bipartition, the Heisenberg interaction on a bipartite lattice can be made sign-problem-free. On a non-bipartite lattice, if this transformation is carried out given some bipartition, the model still retains a sign problem due to \(H^{ij}_2\) on bonds connecting sites in the same sublattice.

For \(S = \frac{1}{2}\), the Heisenberg interaction after the above unitary transformation can be written as
\[
H^{ij}_2 = \frac{J}{2} \left( |\uparrow_i^z \downarrow_j^z\rangle \langle \uparrow_i^z \downarrow_j^z| + |\downarrow_i^z \uparrow_j^z\rangle \langle \downarrow_i^z \uparrow_j^z| + |\uparrow_i^z \uparrow_j^z\rangle \langle \uparrow_i^z \uparrow_j^z| + |\downarrow_i^z \downarrow_j^z\rangle \langle \downarrow_i^z \downarrow_j^z| \right) \tag{7}
\]
with \(|\uparrow_i^z, \downarrow_j^z\rangle\) denoting the \(S^z\) eigenstates at site \(i\). The nearest neighbour Heisenberg Hamiltonian can now be written as a sum on bond operators:
\[
H = \sum_{\langle ij \rangle} H^{ij}_2 = \sum_b H_b. \tag{8}
\]
The powers of \(H\) in eq. (2) can then be replaced by a sum on product strings of two-body operators, \(H_{b_1}H_{b_2} \ldots H_{b_n}\). If \(S_n\) denotes a string of operator indices, the partition function becomes
\[
Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{S_n} \langle \alpha | H_{b_1} H_{b_2} \ldots H_{b_n} | \alpha \rangle. \tag{9}
\]
The “computational” basis states, \(\alpha\), are usually chosen as the tensor product states as follows:
\[
|\alpha\rangle = |S_0\rangle \otimes |S_1\rangle \otimes |S_2\rangle \otimes \cdots \tag{10}
\]
with \(S_i \in \{\uparrow_i^z, \downarrow_i^z\}\). The bond operators, \(H_b\), are generally chosen such that the action of the operator on one basis state gives an unique basis state and not a linear combination of basis states, i.e., \(H_b|\alpha\rangle = |\alpha'\rangle\), with \(|\alpha\rangle\) and \(|\alpha'\rangle\) both being \(S^z\) basis states. This is done by separating the diagonal and off-diagonal operator pieces of \(H^{ij}_2\), i.e., the index \(b\) does not just refer to the bond location, but also for distinguishing a diagonal operator action from an off-diagonal operator action in eq. (7). This so-called “no branching” condition [2] ensures that the successive action of operators in the operator string on \(|\alpha\rangle\) yields a unique sequence of states in “imaginary time”. Thus, the sum on all sequences of spin states in eq. (3) is replaced by an equivalent sum on operator strings. Sampling spin configurations corresponding to eq. (9) can be shown to be equivalent to sampling closely-packed coloured loop configurations in one higher dimension [2]. For certain models, like rotationally symmetric \(S = \frac{1}{2}\) models, every operator string corresponds to a unique loop configuration and vice versa as shown in the left panel of figure 1. Each
of the loops in the closely-packed coloured loop configuration can be coloured independently. The number of colours the loops can take is equal to the number of ways one can “colour” a spin or the basic degree of freedom that lives on the lattice sites. In the present case, the spins can have two states, \(|\uparrow\rangle\) or \(|\downarrow\rangle\), and therefore the loops can have two colours.

We may then rewrite the partition function as

\[
Z = \sum_{\{C_{\text{loops}}\}} \sum_{\{\alpha\}} W(C_{\text{loops}}). \tag{11}
\]

Here \(C_{\text{loops}}\) is any allowed closely-packed uncoloured loop-gas configuration with only one underlying operator where two loops abut each other at various (imaginary) time slices (figure 1, right). The weight of each such configuration is given by \(W(C_{\text{loops}})\), where

\[
W(C_{\text{loops}}) = \frac{1}{n!} \left(\frac{\beta J}{2}\right)^n. \tag{12}
\]

\(\{\alpha\}\) is a set of colours for the loops. The left panel of figure 1 shows one example from this set. If there are \(n_l\) loops in the configuration, the sum over \(\{\alpha\}\) is over \(2^{n_l}\) coloured configurations corresponding to the independent ways of colouring all the loops. The SSE algorithm involves sampling the coloured loop configurations according to their weights. Changing the colour of a loop leads to a non-local update (sometime called an “operator loop” update or just a loop update) in the QMC configuration which makes the SSE approach quite powerful.

For rotationally-symmetric Hamiltonians like the Heisenberg antiferromagnet where the matrix elements corresponding diagonal Hamiltonian operator actions and off-diagonal Hamiltonian operator actions are equal (e.g. as in eq. (9)), we may go one step further and resum over the spin or colour values of these closely-packed loops without breaking or changing any loop connections in the operator string. This then renders the ensemble as a configuration of closely-packed uncoloured loops as shown in the right panel of figure 1. This loop-gas representation for the high-temperature series may be written as

\[
Z(\beta) = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{s_n} 2^n (h_{b_1}h_{b_2} \ldots h_{b_n}), \tag{13}
\]

where the bond index \(b_i\) is now the only indexing required, \(h_{b_i}\) indicates the spin-symmetric matrix element contribution (\(-\frac{J}{2}\) in our example) at \(b_i\), and \(n_l\) is the number of loops in a given configuration. Equation (13) is then modified to

\[
Z = \sum_{\{C_{\text{loops}}\}} W(C_{\text{loops}}), \tag{13}
\]

where \(C_{\text{loops}}\) is as defined earlier, but the weights are modified to \(W(C_{\text{loops}}) = \frac{2^n}{n!} \left(\frac{\beta J}{2}\right)^n\).

The algorithm to sample uncoloured loop configurations was dubbed as the resummed-SSE (RSSE) algorithm [3]. This has some advantages over the standard or coloured SSE algorithm. In [3], we demonstrated it to be naturally advantageous in simulating quantum paramagnetic phases where coloured SSE can face ergodicity problems. It has also been shown in previous work that partial resummation can be used as an approach to reduce or solve the sign problem for certain models in world-line loop algorithms [4,5] which is a closely-related algorithm to SSE [1]. In these models, when one flips the colour of certain coloured loops, it changes the overall sign of the QMC configuration without changing its weight. Such loops were called “merons”. Resumming over merons can eliminate the sign problem in certain models. In §3.1, we describe one quantum spin model (perhaps the only) where this technique has been shown to be successful in eliminating the sign problem for certain observables and minimizing it in others. This technique cannot be blindly applied to models on canonical geometrically frustrated lattices because these algorithms are often not ergodic on such lattices as we will see through examples. In §3.2, we describe how this ergodicity problem can be remedied using the RSSE algorithm. It can thus be used to simulate the Heisenberg model on canonical geometrically frustrated lattices ergodically. However, this still has a severe sign problem. In §3.3, we explore a possible approach to reduce the sign problem on these lattices based on meron resummation and explain why it does not work.

3. Sign-problem discussion

3.1 Meron resummation

Consider the following XXZ Hamiltonian, with a ferromagnetic coupling in the \(z\)-direction and an
antiferromagnetic coupling in the $xy$-plane:

$$H = - \sum_{\langle ij \rangle} (S_i^x S_j^x - S_i^y S_j^y - S_i^z S_j^z). \tag{14}$$

This model has positive off-diagonal matrix elements. In terms of brief describe now. Using this concept, the model can actually be simulated in the original basis. On a geometrically frustrated lattice, this model has a severe sign problem even though the ferromagnetic Hamiltonian is not frustrated. One way to remedy the sign problem is to change the basis [5]. By a trivial relabeling such that the ferromagnetic Hamiltonian is not frustrated. This model has positive off-diagonal matrix elements.

This is equivalent to the Heisenberg ferromagnet on a bipartite lattice up to an unitary transformation on one sublattice of the bipartition. On a geometrically frustrated lattice, this model has a severe sign problem even though the ferromagnetic Hamiltonian is not frustrated. One way to remedy the sign problem is to change the basis [5]. By a trivial relabeling such that the ferromagnetic coupling is in the $y$-direction, we get

$$H = - \sum_{\langle ij \rangle} (S_i^y S_j^y - S_i^x S_j^x - S_i^z S_j^z). \tag{15}$$

Now working in the basis where $S^x$ is diagonal, we define $S^+ = S^x + i S^z$ and $S^- = S^y - i S^z$. $H$ can be written, up to a constant, as

$$H = - \sum_{\langle ij \rangle} \left[ \left( \frac{1}{4} - S_i^x S_j^x \right) + \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) \right]. \tag{16}$$

This can be rewritten in terms of $S^x$ basis states as

$$H = - \frac{1}{2} \sum_{\langle ij \rangle} \left( | \uparrow_i \downarrow_i \uparrow_j \downarrow_j \rangle \langle \uparrow_i \downarrow_i \uparrow_j \downarrow_j | + | \downarrow_i \uparrow_i \downarrow_j \uparrow_j \rangle \langle \downarrow_i \uparrow_i \downarrow_j \uparrow_j | + | \uparrow_i \downarrow_i \uparrow_j \downarrow_j \rangle \langle \downarrow_i \uparrow_i \downarrow_j \uparrow_j | + | \downarrow_i \uparrow_i \downarrow_j \uparrow_j \rangle \langle \uparrow_i \downarrow_i \uparrow_j \downarrow_j | \right). \tag{17}$$

All matrix elements are negative, hence this is now a sign-problem-free model. The loop moves in the operator loop update for this model are shown in figure 2. Another solution to the sign problem using the concept of a “meron” or sign-changing loop was given by Henelius and Sandvik on the square lattice with nearest and next-nearest neighbour interactions [5] which we briefly describe now. Using this concept, the model can actually be simulated in the original basis. In terms of $S^z$ basis states, $H$ can be written, up to a constant, as

$$H = - \frac{1}{2} \sum_{\langle ij \rangle} \left( | \uparrow_i \downarrow_i \uparrow_j \downarrow_j \rangle \langle \uparrow_i \downarrow_i \uparrow_j \downarrow_j | + | \downarrow_i \uparrow_i \downarrow_j \uparrow_j \rangle \langle \downarrow_i \uparrow_i \downarrow_j \uparrow_j | + | \uparrow_i \downarrow_i \uparrow_j \downarrow_j \rangle \langle \downarrow_i \uparrow_i \downarrow_j \uparrow_j | + | \downarrow_i \uparrow_i \downarrow_j \uparrow_j \rangle \langle \uparrow_i \downarrow_i \uparrow_j \downarrow_j | \right). \tag{18}$$

Consider the following two-spin $XXZ$ interaction on a frustrated lattice built out of triangular motifs

$$H_{XXZ}^{ij} = S_i^z S_j^z - S_i^x S_j^x - S_i^y S_j^y. \tag{19}$$

This is the negative of the interaction in eq. (14) which implies that this model has all the negative off-diagonal matrix elements. Therefore it is sign-problem-free. It can be written as

$$H_{XXZ}^{ij} = - \frac{1}{2} (| \uparrow_i \downarrow_i \uparrow_j \downarrow_j \rangle \langle \uparrow_i \downarrow_i \uparrow_j \downarrow_j | + | \downarrow_i \uparrow_i \downarrow_j \uparrow_j \rangle \langle \downarrow_i \uparrow_i \downarrow_j \uparrow_j | + | \uparrow_i \downarrow_i \uparrow_j \downarrow_j \rangle \langle \downarrow_i \uparrow_i \downarrow_j \uparrow_j | + | \downarrow_i \uparrow_i \downarrow_j \uparrow_j \rangle \langle \uparrow_i \downarrow_i \uparrow_j \downarrow_j | ). \tag{20}$$

Naively, this can be simulated without a sign problem on a non-bipartite lattice. However, the standard SSE algorithm is not ergodic in simulating this model on a geometrically frustrated lattice. This can be seen by simulating the following model on a frustrated chain:

$$H = \sum_{\langle ij \rangle} H_{XXZ}^{ij} + g \sum_{\langle ij \rangle} H_{XXZ}^{ij}. \tag{21}$$

By comparing the energy observable per unit site for different parameters as given in table 1, the lack of ergodicity is seen clearly. Compare the third and fourth

![Figure 2. Loop moves in the operator loop update for the model in eq. (17).](Image)

![Figure 3. Loop moves in the operator loop update for the model in eq. (18).](Image)
Table 1. Comparison of energy per unit site, $e_1$, of model in eq. (21) for $L = 8$ calculated from exact diagonalization (ED), SSE and RSSE. The SSE values clearly do not match ED but RSSE values do. $e_2$ denotes energy per unit site of the model in eq. (21), where $H_{XXZ}^{ij}$ is replaced by eq. (23), using SSE. Comparison with ED shows that this model gives correct results.

| $g$ | $\beta$ | $e_1$ (ED)  | $e_1$ (SSE)  | $e_1$ (RSSE)  | $e_2$ (SSE)  |
|-----|---------|-------------|-------------|-------------|-------------|
| 0.1 | 1.0     | −0.485421   | −0.4774(2)  | −0.4854(4)  | −0.4858(6)  |
| 0.5 | 1.0     | −0.647273   | −0.6105(2)  | −0.6473(4)  | −0.6476(6)  |
| 1.0 | 1.0     | −0.938847   | −0.8769(4)  | −0.9387(4)  | −0.9378(7)  |

columns of table 1. The standard SSE loop update is unable to generate certain configurations in the configuration space of this model. These are configurations with an odd number of off-diagonal operators (an example of such a configuration is shown in figure 4). The SSE updates principally involve two steps: (1) a diagonal update, involving insertion and removal of diagonal operators, and (2) the operator loop update that converts diagonal operators into off-diagonal operators and vice versa. In this model, any loop has to touch an even number of operators in order for it to close. Since, an even number is either the sum of two even numbers or two odd numbers, therefore flipping a loop can only make an even number of diagonal operators into off-diagonal operators (and vice versa) or an odd number of diagonal operators into off-diagonal operators (and vice versa). In other words, the loop update cannot change the parity of the count of off-diagonal operators in any configuration. One generally starts with a configuration consisting of all diagonal operators, from which it is impossible to generate a configuration consisting of an odd number of off-diagonal operators with standard SSE updates. Generally speaking, this is how ergodicity gets violated by being stuck in one of these parity sectors more. This problem can be circumvented by a change of basis similar to the one in the previous section:

$$H_{XXZ}^{ij} = -\left(\frac{1}{4} + S_i^z S_j^z\right) - (S_i^x S_j^x - S_i^y S_j^y)$$

$$= -\left(\frac{1}{4} + S_i^z S_j^z\right) - \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) \tag{22}$$

In terms of the $S^z$ basis states, this can be written as

$$H_{XXZ}^{ij} = -\frac{1}{2}( | \uparrow_i \uparrow_j \rangle \langle \uparrow_i \uparrow_j | + | \downarrow_i \downarrow_j \rangle \langle \downarrow_i \downarrow_j |$$

$$+ | \uparrow_i \downarrow_j \rangle \langle \downarrow_i \uparrow_j | + | \downarrow_i \uparrow_j \rangle \langle \uparrow_i \downarrow_j | ) \tag{23}$$

This model is fully ergodic on frustrated lattices and does not suffer from a sign problem. This is because for this model there cannot be configurations with an odd number of off-diagonal operators similar to the example in figure 4. In fact, the example in figure 4 is the geometric space-time primitive or base case required to have an odd number of off-diagonal operators in any configuration for models with two-site Heisenberg terms in the Hamiltonian. Any model which is not compatible with such a space-time primitive will not have an odd number of off-diagonal operators. Thus, only the even parity sector is involved here, and thus the operator loop update can sample it ergodically. See the sixth column of table 1.

Another solution to simulate the model in the $S^z$ basis itself is to use RSSE which overcomes the ergodicity limitation of SSE. In RSSE, there is no notion of diagonal and off-diagonal operators as we saw in §2, which effectively makes this algorithm ergodic in sampling both parity sectors for the off-diagonal operator counts. If one carries out resummation-based updates which are colour-blind and then colours in the loops, one can easily generate configurations as shown in figure 4 and others with an odd number of off-diagonal operators. See the fifth column of table 1. It may be pointed out that even though a basis transformation can eliminate the sign problem in some cases (as in the
Table 2. Comparison of energy per unit site, $e$, of model in eq. (24) for $L = 8$ calculated from ED and RSSE. The statistical estimation error shoots up as the average sign rapidly falls to zero as the temperature is reduced.

| $g$ | $\beta$ | $e$ (ED) | $e$ (RSSE) | Avg. sign |
|-----|---------|---------|-----------|-----------|
| 1.0 | 1.0     | -0.776879 | -0.77683(9) | 0.6170(1) |
| 1.0 | 2.0     | -0.892962 | -0.8926(4)  | 0.09809(9) |
| 1.0 | 3.0     | -0.95662  | -0.958(2)   | 0.0138(1)  |
| 1.0 | 4.0     | -0.990501 | -1.01(2)    | 0.0025(2)  |

previous sub-section) or fix ergodicity issues (as in this sub-section), however, there is still an added value in having the ability to simulate in the original basis (as in both these sub-sections). This is because it makes the measurements of correlation functions in both the direction of the quantization axis and perpendicular to it especially convenient.

3.3 Resummation vis-à-vis the sign problem due to geometric frustration

Consider finally the following Hamiltonian:

\[ H = \sum_{\langle ij \rangle} H_{ij}^2 + g \sum_{\langle\langle ij \rangle\rangle} H_{ij}^2 \] (24)

involving just antiferromagnetic Heisenberg terms as defined in eq. (6). Here, the interaction of eq. (6) is summed over nearest-neighbour bonds and the next-nearest-neighbour bonds of a 1d chain. This chain model is thus a geometrically frustrated system. If we label the even and odd sites on the chain as A and B, the unitary transformation on A sites (say), $S_x^A \rightarrow -S_x^A$ and $S_y^A \rightarrow -S_y^A$, does not make the model sign-problem-free. For an AB bond, the interaction can be written in the $S_z$ basis as in eq. (7) which is sign-problem-free. For an AA bond, the off-diagonal terms change sign:

\[ H_{ij}^{AA} = -\frac{J}{2} \left( | \uparrow_i \downarrow_j \rangle \langle \downarrow_i \uparrow_j | + | \downarrow_i \uparrow_j \rangle \langle \uparrow_i \downarrow_j | \right) \]

Thus, the sign problem still remains due to off-diagonal operators on AA bonds coming from QMC configurations with an odd number of such AA off-diagonal operator contributions as in the example of figure 4. In a similar vein to §3.2, RSSE can sample this QMC ensemble ergodically as shown in table 2, while standard SSE updates do not ergodically sample both parity sectors for the off-diagonal operator counts.

Let us hypothetically have a loop in the QMC configuration that touches an odd number of AA bond operators (if the loop touches the same AA bond operator twice, it is counted as 2). When one flips the colour of such a loop, the off-diagonal operators become diagonal and vice versa. Since (1) an odd number is always a sum of an even and an odd number, and (2) the operators on the AA bonds change sign while undergoing a change from diagonal action to off-diagonal action or vice versa, therefore, the weight of the full QMC configuration changes sign under such a colour flip. As discussed previously, such loops that change sign upon colour flips can serve as merons [5], in this context. If such loops were to exist, they can be resummed away to reduce the sign problem in simulations of this model, as has been described before for a semi-frustrated model in §3.1.

Such loops, however, do not exist in the QMC configuration space of eq. (24) as can be explicitly checked in simulations. This is also the case for other geometrically frustrated lattices like the triangular lattice, the Kagome lattice, etc. This can be understood by providing the loops with an orientation. When one starts to grow a loop, the direction of the loop switches when an operator is encountered (see figures 4 and 5). Encountering an AB bond also switches the sublattice along with the direction, therefore it is clear that the loop has to encounter an even number of AB bond operators to come back to the same sublattice it started with in order to close the loop. If the model had only AB bonds (as
in the bipartite case), the loop will be oriented in one direction on the A sublattice and in the opposite direction on the B sublattice. Therefore, when the loop comes back to the point it started, it automatically ensures that it does with the same orientation as the one it started with, since the orientation is determined by the sublattice of the starting point. Note that loops do not retrace themselves in this model and many-related Heisenberg models. In the presence of AA bond operators, the orientation is not determined by the sublattice any more. These bonds reverse the direction of the loop on the same sublattice (see figure 5). Therefore, in order to ensure that the direction of the loop is reversed twice on the same sublattice to close the loop, it is required to touch an even number of AA bond operators. This forbids the hypothesized merons thus precluding a meron resummation strategy to reduce the sign problem in canonical geometrically frustrated lattices.

However, as seen in this sub-section and the previous one, it is noteworthy that RSSE gives us the facility to ergodically sample both parity sectors of off-diagonal processes on frustrated lattice with triangular motifs for Hamiltonians where such quantum processes are at play.

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