Generalization of the singlet sector valence-bond loop algorithm to antiferromagnetic ground states with total spin $S_{\text{tot}} = 1/2$

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Abstract. We develop a generalization of the singlet sector valence-bond basis projection algorithm of Sandvik, Beach, and Evertz (Sandvik 2005 Phys. Rev. Lett. 95 207203; Beach and Sandvik 2006 Nucl. Phys. B 750 142; Sandvik and Evertz 2010 Phys. Rev. B 82 024407) to cases in which the ground state of an antiferromagnetic Hamiltonian has total spin $S_{\text{tot}} = 1/2$ in a finite-size system. We explain how various ground state expectation values may be calculated by using generalizations of the estimators developed in the singlet case, and illustrate the power of the method by calculating the ground state spin texture and bond energies in an $L \times L$ Heisenberg antiferromagnet with $L$ odd and free boundaries.

Keywords: spin chains, ladders and planes (theory), spin liquids (theory), quantum Monte Carlo simulations
1. Introduction

Understanding the ground states of strongly correlated condensed matter systems is a central problem in computational physics. Several approaches have achieved a degree of success in this endeavor. These include various sophisticated quantum Monte Carlo (QMC) techniques for sampling the partition function \( \text{Tr}(\exp(-H/T)) \) of a system with Hamiltonian \( H \) at temperature \( T \), and using this sampling procedure to estimate the thermal expectation values of various operators \( \langle \hat{O} \rangle_T = \text{Tr}(\hat{O}\exp(-H/T))/(\text{Tr}(\exp(-H/T))) \) [4]–[6]. Although these can be used for relatively large finite-size systems, they are intrinsically finite-temperature methods and accessing the very low temperature regime involves doing calculations at successively lower temperatures and then extrapolating.

Other approaches include various exact diagonalization techniques that obtain the lowest energy state in a given sector. These are severely constrained by memory requirements in terms of the system sizes that they can handle. While this problem can be overcome in one dimension by the sophisticated density matrix renormalization group method [7], there is as yet no generalization of this method that works equally well in higher dimension, although there has been considerable progress recently [8].

Recently, Sandvik and collaborators have developed an extremely elegant and sophisticated projection algorithm [1]–[3] that essentially solves the problem of calculating the ground state expectation values of quantities in a large class of \( S = 1/2 \) antiferromagnetic spin systems which have the ground state in the total spin \( S_{\text{tot}} = 0 \) singlet sector. This singlet sector algorithm works in the ‘bipartite valence-bond’ basis for singlet states (see below), and exploits the overcompleteness of this basis to develop a procedure [2] for evaluating the expectation values of some observables \( \mathcal{O} \) for the (unnormalized) ground state \( |\psi_g\rangle = (-H)^m|s\rangle \) obtained by acting on an arbitrary singlet state \( |s\rangle \) with a large power of \(-H\). The key to its success is an extremely efficient [3] procedure for stochastically sampling \( \langle s|(-H)^m\mathcal{O}(-H)^m|s\rangle/\langle s|(-H)^{2m}|s\rangle \), which allows one to handle large systems with as many as \( 10^4 \) spins in favorable cases.
The ground state spin of a finite system made up of spin-half variables interacting antiferromagnetically naturally depends on the nature of the finite sample: if the total number of spin-half variables is even, one expects a ground state in the singlet sector, while systems with an odd number of spins will have a ground state in the total spin \( S_{\text{tot}} = 1/2 \) sector. For instance, an \( L \times L \) square lattice Heisenberg antiferromagnet with periodic boundary conditions and \( L \) even will have a singlet ground state, while the same magnet with \( L \) odd and free boundaries will have a ground state spin of \( S_{\text{tot}} = 1/2 \). In many situations, it is useful to be able to handle both kinds of finite systems. For instance, if one wants to model experiments that dope insulating antiferromagnets with non-magnetic ions like Zn [9,10] that substitute for the magnetic moments, it is convenient to study \( L \times L \) periodic systems with \( L \) even as before, but with one spin removed from the system to model the missing-spin defect introduced by Zn doping.

The original valence-bond projector loop algorithm [1,3] allows one to study the singlet sector ground states of systems with an even number of spins. Here we ask whether it is possible to come up with an analogous procedure for the total spin \( S_{\text{tot}} = 1/2 \) sector of systems with an odd number of spins in order to compute properties of the \( S_{\text{tot}} = 1/2 \) doublet ground state of antiferromagnetic systems with an odd number of spin-half variables interacting antiferromagnetically. As our results demonstrate, the answer turns out to be very satisfying: using a judiciously chosen basis for the \( S_{\text{tot}} = 1/2 \) sector of such systems, we find that is indeed possible to construct an analogous procedure that works as well in the total spin \( S_{\text{tot}} = 1/2 \) sector as the original singlet sector algorithm of Sandvik and collaborators [1]–[3]. Here we detail several aspects of this generalization. To illustrate the power of the method, we also show results for the ground state ‘spin texture’ in the \( S^z_{\text{tot}} = 1/2, S_{\text{tot}} = 1/2 \) ground state of an \( L \times L \) square lattice \( S = 1/2 \) Heisenberg antiferromagnet with open boundary conditions and \( L \) odd and as large as \( L = 101 \).

2. Basis

A judicious choice of basis is the key to generalizing the original singlet sector valence-bond projector loop QMC algorithm to the study of bipartite spin-half antiferromagnets with \( N_B \) B-sublattice sites, \( N_A = N_B + 1 \) A-sublattice sites, and a doublet ground state in the \( S_{\text{tot}} = 1/2 \) sector. While other choices may also be possible, we find it convenient to use the basis

\[
\{ |A, a_f \sigma \rangle \} \equiv \{ |[A(b_1)b_1], [A(b_2)b_2] \cdots [A(b_{N_B})b_{N_B}]; a_f \sigma \rangle \}. \tag{1}
\]

Each member of this basis has one A-sublattice spin \( S_{a_f} \) in either the \( |a_f \sigma = \uparrow \rangle \equiv |S_{a_f}^z = +1/2 \rangle \) or the \( |a_f \sigma = \downarrow \rangle \equiv |S_{a_f}^z = -1/2 \rangle \) state along the quantization axis \( \hat{z} \), while the \( N_B \) spins \( S_{b_i} \) on the B-sublattice sites each form a singlet state (‘valence bond’)

\[
|[A(b_i)b_i]\rangle = \frac{(|[A(b_{\uparrow\downarrow})\uparrow\downarrow, b_{\downarrow\uparrow} \downarrow\uparrow] - |[A(b_{\downarrow\uparrow})\downarrow\uparrow, b_{\uparrow\downarrow}\uparrow\downarrow])}{\sqrt{2}} \tag{2}
\]

with a partner \( S_{A(b_i)} \) on the A-sublattice. All basis states are obtained by allowing all possible \( a_f \), two choices for \( \sigma \), and all possible ‘matching’ functions \( A \) consistent with a given choice of ‘free spin’ \( a_f \). Note that this basis set is actually a union of two distinct

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basis sets

\[ \{ | A, a_f \uparrow \rangle \} \equiv \{ [ | A(b_1) b_1, A(b_2) b_2 \cdots \{ A(b_{N_B}) b_{N_B} \}; a_f \uparrow \} \} \quad (3) \]

corresponding to the two allowed choices for the conserved quantum number \( S^z_{\text{tot}} \) in the \( S_{\text{tot}} = 1/2 \) sector of an \( SU(2) \) invariant composed of an odd number of spin-1/2s.

This basis is (over)complete in a manner entirely analogous to the bipartite valence-bond basis that was used in the original singlet sector algorithm [2,3]. This may be seen as follows: consider adding one extra B-sublattice site \( b_{N_B + 1} \) to our system to make the total number of spins even. The singlet sector of this larger system is spanned by the (over)complete bipartite valence-bond basis. States in this basis are in one-to-one correspondence with possible pairwise matchings \( \mathcal{P} \) that ‘find’ an A-sublattice ‘partner’ \( \mathcal{P}(b_i) \) for each B-sublattice site \( b_i \) to form a singlet:

\[ | \mathcal{P} \rangle \equiv | \mathcal{P}(b_1) b_1, \mathcal{P}(b_2) b_2 \cdots | \mathcal{P}(b_{N_B + 1} b_{N_B + 1}) \rangle \]. \quad (5) \]

Now, by the laws of angular momentum addition, singlet states of the larger system can only arise from tensor products of the additional spin-half variable at site \( b_{N_B + 1} \) with the \( S_{\text{tot}} = 1/2 \) states of the smaller system. Therefore, to check for (over)completeness of our proposed basis for the smaller system, we only need to check whether all states in the bipartite valence-bond basis of the larger system are obtainable as tensor products of states of the additional spin \( S_{b_{N_B + 1}} \) with states in our proposed \( S_{\text{tot}} = 1/2 \) basis. This is certainly the case, as is readily seen by identifying \( a_f \) with \( \mathcal{P}(b_{N_B + 1}) \) and \( A \) with the restriction of \( \mathcal{P} \) to the domain \( (b_1, b_2, \ldots b_{N_B}) \). Our proposed basis is thus overcomplete in a manner entirely analogous to the original bipartite valence-bond basis for the singlet sector.

In practice, for \( SU(2) \) symmetric spin Hamiltonians of interest to us here, we will additionally exploit the conservation of the \( z \) component of spin and restrict attention to the basis \( \{ | A(b_1) b_1, A(b_2) b_2 \cdots \{ A(b_{N_B}) b_{N_B} \}; a_f \uparrow \} \} \) that only spans the \( S^z_{\text{tot}} = 1/2, S_{\text{tot}} = 1/2 \) sector a system with \( N_A = N_B + 1 \) spin-1/2s on the A-sublattice, and \( N_B \) spin-1/2s on the B-sublattice.

3. Overlaps and operators

We now indicate the changes that arise in the formulas for the wavefunction overlaps between basis states, and for the action of exchange operators when working in the \( S_{\text{tot}} = 1/2 \) sector. As is well known, the wavefunction overlaps between two bipartite VB basis states \( | \mathcal{P} \rangle \) and \( | \mathcal{P}' \rangle \) of the singlet sector basis are determined by the number of cycles needed to go from the permutation \( \mathcal{P} \) to the permutation \( \mathcal{P}' \). More pictorially, one may consider the overlap diagram of the two valence-bond covers viewed as ‘complete dimer covers’ or ‘perfect’ matchings. This overlap diagram contains \( N_{\text{loop}} \) (closed) loops of various lengths \( l_\mu \), such that each site is part of exactly one loop (see figure 1). Knowing this overlap diagram, one may calculate the corresponding wavefunction overlap to be

\[ \langle \mathcal{P} | \mathcal{P}' \rangle = 2^{N_{\text{loop}} + N_s/2}, \text{ where } N_s \text{, the total number of spins, is assumed even.} \]
Generalization of the singlet sector valence-bond loop algorithm

Generalizing this to states in our basis for the $S_{\text{tot}} = 1/2$ sector, we note that the corresponding picture is now in terms of the overlap diagram of two partial valence-bond covers $(A, a_f)$ and $(A', a'_f)$, each of which leaves one site free (uncovered by a valence bond). Such an overlap diagram necessarily involves exactly one ‘open string’ of length $l_f$ connecting $a_f$ to $a'_f$, in addition to $N_{\text{loop}}$ (closed) loops of various lengths $l_\alpha$ (see figure 1).

An elementary calculation reveals that the wavefunction overlap in our $S_{\text{tot}} = 1/2$ case is given as

$$\langle A a_f \sigma | A' a'_f \sigma' \rangle = \delta_{\sigma \sigma'} 2^{N_{\text{loop}} / 2} / 2^{(N_s - 1)/2},$$

with $N_s$, the number of sites, now taken to be odd.

The original singlet sector algorithm relies heavily [1]–[3] on a particularly simple action of operators $P_{ij} = \eta_i \eta_j S_i \cdot S_j + 1/4$ on basis states $|P\rangle$. Here $\eta_i = +1$ ($\eta_i = -1$) for $i$ belonging to the A-sublattice (B-sublattice), and thus, the operator $P_{a_i b_j}$ that connects an A-sublattice site $a_i$ to a B-sublattice site $b_j$ is precisely the projection operator that projects to the singlet state of the two spins $S_{a_i}$ and $S_{b_j}$. Our key observation, which allows us to generalize this algorithm to the $S_{\text{tot}} = 1/2$ case, is that the action of $P_{ij}$ on states in our $S_{\text{tot}} = 1/2$ basis remains simple. This is seen as follows: if neither $i$ nor $j$ corresponds to the ‘free’ spin, $P_{ij}$ acts exactly as in the earlier singlet sector case (figures 1(a) and (b)):

\[
\begin{align*}
P_{A(b_a) b_a} \cdots [A(b_a) b_a] \cdots a_f \uparrow &= [\cdots [A(b_a), b_a] \cdots a_f \uparrow], \\
P_{A(b_a) b_b} [\cdots [A(b_a), b_b] [A(b_b), b_b] \cdots a_f \uparrow] &= \frac{1}{2} [\cdots [A(b_a), b_b] [A(b_b), b_a] \cdots a_f \uparrow], \\
P_{A(b_a) A(b_b)} [\cdots [A(b_a), b_a] \cdots [A(b_b), b_b] \cdots a_f \uparrow] &= \frac{1}{2} \cdots [A(b_a), b_b] [A(b_b), b_a] \cdots a_f \uparrow, \\
P_{b_b b_b} [\cdots [A(b_a), b_a] \cdots [A(b_b), b_b] \cdots a_f \uparrow] &= \frac{1}{2} \cdots [A(b_a), b_b] [A(b_b), b_a] \cdots a_f \uparrow.
\end{align*}
\]

(6)

On the other hand, if either $i$ or $j$ corresponds to the free site $a_f$, one can easily check

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that the following holds (figures 1(c) and (d)):

\[
P_{a_f b_a} \cdots [A(b_a) b_a] \cdots a_f \uparrow = \frac{1}{2} \cdots [a_f, b_a] \cdots [A(b_a) \uparrow],
\]

\[
P_{a_f} [A(b_a)] \cdots [A(b_a) b_a] \cdots a_f \uparrow = \frac{1}{2} \cdots [a_f, b_a] \cdots [A(b_a) \uparrow].
\]  

(7)

Thus \( P_{ij} \) either causes no change or rearranges exactly one pair of valence bonds to give a new basis state with amplitude 1/2, or re reconnects one valence bond to move the free spin to give a new basis state, again with amplitude 1/2. The important thing to note is that these rules are in complete analogy to the original singlet sector case.

By analogy to the original singlet sector work [1]–[3], this allows us to formulate a convenient prescription for the calculation of \( \langle A' a'_f | P_{ij} | A a_f \uparrow \rangle \), between two of our basis states, by writing \( \langle A' a'_f | P_{ij} | A a_f \uparrow \rangle = W_{ij} \langle A' a'_f \uparrow \rangle | A a_f \uparrow \rangle \) and developing rules for the weight \( W_{ij} \) by comparing the overlap diagram of \( \langle A' a'_f \uparrow \rangle \) and \( \langle P_{ij} | A a_f \uparrow \rangle \) with the original overlap diagram of \( \langle A' a'_f \uparrow \rangle \) and \( \langle A a_f \uparrow \rangle \). If the action of \( P_{ij} \) makes no changes in the original overlap diagram, \( W_{ij} = 1 \). In addition, \( W_{ij} = 2 \times 1/2 = 1 \) if a loop is split into two loops or the open string is split into one loop and another open string; here, the factor of 2 comes from the fact that the number of loops in the overlap diagram increases by 1, while the factor of 1/2 has its origins in the reconnection amplitude of 1/2 in equations (7). On the other hand, if two loops fuse into one, or if the open string fuses with a loop to give a larger open string, then \( W_{ij} = (1/2) \times (1/2) \), where the first factor of 1/2 reflects the fact that the number of loops is reduced by 1, while the second factor of 1/2 comes from the reconnection amplitude in equation (7). These rules are tabulated in figure 2, and the important thing to note is that the open string can be treated on an equal footing with (closed) loops in all cases, allowing one to generalize the singlet sector rules directly to the \( S_{tot} = 1/2 \) sector case discussed here.

4. Generalization of the Sandvik–Evertz algorithm

With all of this in hand, it is now easy to see that the singlet sector algorithm of Sandvik and collaborators [1]–[3] generalizes straightforwardly to the \( S_{tot} = 1/2 \) sector case for Hamiltonians of the form \( H = -\sum b H_b \), where each piece \(-H_b\) of the Hamiltonian is a projector \( P_{b_1 b_2} \) acting on bond \( b \) connecting spins \( b_1 \) and \( b_2 \). We start with an arbitrary \( S_{tot} = 1/2 \), \( S^z_{tot} = 1/2 \) state \( |\psi_{1/2}| \), say \( |\psi_{1/2}| = |A a_f \rangle \). As in the original singlet sector algorithm, we wish to stochastically sample \( \langle \psi_{1/2} | (-H)^{2m} | \psi_{1/2} \rangle \) by sampling all possible operator strings \( \prod_{\tau=1}^{2m} H_b \) in the decomposition of \( (-H)^{2m} \) into a sum of products, with the weight for each such string being proportional to \( \langle \psi_{1/2} | \prod_{\tau=1}^{2m} H_b | \psi_{1/2} \rangle \). To do this, one splits each \( H_b \) into a term \( H_b^{\sigma=d} \) that is diagonal in the \( \{ S^\tau \} \) eigenbasis, and a term \( H_b^{\sigma=o} \) that is off-diagonal. In addition, one writes \( |\psi_{1/2} \rangle \) in this basis as \( |\psi_{1/2} \rangle = \sum_i (S^\tau_i) C_i \{ S^\tau_i \} |\{ S^\tau_i \} \rangle \). As in the original singlet sector case, each term \( C_i \{ S^\tau_i \} C_j \{ S^\tau_j \} |\{ S^\tau_i \} \rangle \prod_{\tau=1}^{2m} H_b^{\sigma=d} |\{ S^\tau_j \} \rangle \) is generated by working in a ‘space–time’ loop representation and using a combination of ‘diagonal updates’ in which some \( H_b^{\sigma=d} \) is moved to a different bond \( b'_\tau \) and ‘loop updates’ whereby each space–time loop is flipped with probability 1/2; this loop update allows one to switch between diagonal and off-diagonal pieces of a given set of bond operators, while simultaneously sampling all possible spin configurations \( \{ S^\tau_i \} \) in the state at \( \tau = 0 \) and \( \tau = 2m \). The only difference from the original singlet sector case is that we now have precisely one open string in the
space–time diagram, which connects the ‘free spin at \( \tau = 0 \)’, i.e. the unpaired spin in \( |\psi_{1/2}^↑\rangle \), to the ‘free spin at \( \tau = 2m \)’, i.e. the unpaired spin in \( \langle\psi_{1/2}^↑| \), and which cannot be flipped, since the unpaired spins in all of our \( S_{\text{tot}} = 1/2, S_{\text{tot}}^z = 1/2 \) basis states have fixed \( z \) projection of \(+1/2\). Finally, as in the singlet case, we can easily generalize this procedure to treat Hamiltonians that also contain products \( -P_bP_{b'} \) of projectors \( P \) acting on distinct bonds \( b \) and \( b' \) of the lattice.

5. Estimators

As in the singlet sector case [1]–[3], physical properties can be calculated by taking each space–time loop diagram generated by the algorithm and ‘cutting it at \( \tau = m \)’ to obtain the overlap diagram that represents the overlap of \( \prod_{\tau=1}^{m} H_{b_{\tau}}^{\sigma_{\tau}} |\psi_{1/2}| \) with \( \langle\psi_{1/2}| \prod_{\tau=m+1}^{2m} H_{b_{\tau}}^{\sigma_{\tau}} \). Consider for instance the Néel order parameter \( \vec{m}_s = \sum_i \eta_i \vec{S}_i \). Clearly, \( \langle m_x^s \rangle = \langle m_y^s \rangle = 0 \). However, \( \langle m_z^s \rangle \) receives contributions from sites on the open string in the overlap diagram, since the open string, in contrast to (closed) loops, has only one orientation and therefore cannot be flipped. More formally, we may write \( \langle \mathcal{A}' a_{f}^\uparrow \uparrow | S_{i}^{z} | \mathcal{A} a_{f}^\uparrow \uparrow \rangle = W_i \langle \mathcal{A}' a_{f}^\uparrow \uparrow | S_{i}^{z} | \mathcal{A} a_{f}^\uparrow \uparrow \rangle \) and note that \( W_i = \eta_i / 2 \) if \( i \) is part of the open string in the overlap diagram.

Figure 2. Action of a singlet projector on the overlap loops for closed loops ((a), (b)) and open string ((c), (d)). Corresponding weights are given within parenthesis.

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between \((A'a'f)\) and \((Aaf)\) and 0 otherwise. We thus find

\[
\langle m^2 \rangle = \frac{\langle l_f \rangle}{2}
\]

where the angular brackets on the right denote the ensemble average over the ensemble of overlap diagrams generated by the modified \(S_{\text{tot}} = 1/2, S_{\text{tot}}^z = 1/2\) sector algorithm outlined above.

We now turn to \(\langle \tilde{m}_s^2 \rangle = \langle \sum_{ij} (P_{ij} - 1/4) \rangle\). As noted earlier, whenever \(i\) and \(j\) are both in the open string or the same (closed) loop, the corresponding weight \(W_{ij} = 1\), while \(W_{ij} = 1/4\) when \(i\) and \(j\) do not both belong to the open string or the same (closed) loop. For an overlap diagram with closed loops of lengths \(l_\alpha\) (with \(\alpha = 1, 2, \ldots, N_l - 1\)) and an open string of length \(l_N = l_f\), the latter can occur in \(\sum_{\alpha, \beta = 1}^{N_l} l_\alpha l_\beta\) ways where the prime on the sum indicates that \(\alpha = \beta\) is disallowed, while the former can occur in \(\sum_{\alpha = 1}^{N_l} l_\alpha^2\) ways. As in the singlet sector case, we thus obtain

\[
\langle \tilde{m}_s^2 \rangle = \langle \frac{1}{4} \sum_{\alpha, \beta = 1}^{N_l} l_\alpha l_\beta + \sum_{\alpha = 1}^{N_l} l_\alpha^2 - \frac{1}{4} \sum_{\alpha, \beta = 1}^{N_l} l_\alpha l_\beta \rangle
\]

where the angular brackets on the right again indicate average over the ensemble of overlap diagrams generated by the algorithm. This reduces to

\[
\langle \tilde{m}_s^2 \rangle = \left\langle \frac{3}{4} \sum_{\alpha = 1}^{N_l} l_\alpha^2 \right\rangle
\]

where the angular brackets on the right again denote averaging over the ensemble of overlap diagrams generated by the algorithm, and the important thing to note is that this estimator treats the open string \((\alpha = N_l)\) on the same footing as the closed loops \((\alpha = 1, 2, \ldots, N_l - 1)\).

Finally, we consider the ground state expectation value of the fourth power of the Néel order parameter, i.e. \(\langle (\tilde{m}_s^2)^2 \rangle\). To derive the estimator for this in \(S_{\text{tot}} = 1/2, S_{\text{tot}}^z = 1/2\), we follow Sandvik and Beach [2], and write \(\langle (\tilde{m}_s^2)^2 \rangle = \langle \sum_{ij} \sum_{kl} (P_{ij} - 1/4)(P_{kl} - 1/4) \rangle\). As in [2], we note that the estimator for this quantity differs from the square of the estimator for \(\tilde{m}_s^2\) only when the action of \(P_{ij}\) ‘interferes’ with the action of \(P_{kl}\), i.e. when the actual weight \(W_{ijkl} \equiv \langle A'a'_f \uparrow | P_{ij} P_{kl} | Aaf \uparrow \rangle / \langle A'a'_f \uparrow | Aaf \uparrow \rangle \) differs from the product \(W_{ij} W_{kl}\) of the independent weights \(W_{ij} \equiv \langle A'a'_f \uparrow | P_j | Aaf \uparrow \rangle / \langle A'a'_f \uparrow | Aaf \uparrow \rangle\) and \(W_{kl}\) (defined analogously to \(W_{ij}\)). As in the singlet sector case, this happens only in the two cases shown in figure 3, where the difference \(W_{ijkl} - W_{ij} W_{kl}\) has been tabulated. Thus, the only new calculation needed is a count of the number of ways in which each of the cases of figures 3(a)–(d) arise, weighted by the corresponding values of \(W_{ijkl} - W_{ij} W_{kl}\). It is at this step that the open string needs to be treated separately, since we find that this count for a open string in figure 3(c) differs from the analogous count for a closed loop in figure 3(a) by precisely 1: figure 3(a) can arise in \(\frac{1}{3} l_a^4 - \frac{4}{3} l_a^2\) ways, while figure 3(c) can arise in \(\frac{1}{3} l_f^4 - \frac{4}{3} l_f^2 + 1\) ways. On the other hand, both figures 3(b) and (d) arise in precisely \(2l_a^2 l_\beta^2\) ways (with \(l_\beta \equiv l_f\)) for figure 3(d).

With all this in hand, we obtain

\[
\langle (\tilde{m}_s^2)^2 \rangle = \left\langle \left( \frac{3}{4} \sum_{\alpha = 1}^{N_l} l_\alpha^2 \right)^2 \right\rangle + \frac{6}{10} \sum_{\alpha, \beta = 1}^{N_l} \langle l_\alpha^2 l_\beta^2 \rangle - \frac{1}{4} \sum_{\alpha = 1}^{N_l} \langle l_\alpha^4 - 4l_\alpha^2 \rangle - \frac{3}{17}
\]

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which reduces to

$$\langle (\vec{m}_s^2)^2 \rangle = \sum_{\alpha=1}^{N_l} \left( -\frac{5}{8} l_\alpha^4 + l_\alpha^2 \right) + \frac{15}{16} \left( \sum_{\alpha=1}^{N_l} l_\alpha^2 \right)^2 - \frac{3}{4}. \quad (11)$$

Again, the thing to note is that the presence of the open string only changes the estimator by the addition of a constant $$(-\frac{3}{4})$$ when compared to the corresponding expression in the singlet sector case [2].

6. Benchmarks, illustrative results and outlook

To benchmark the method, we focus on an $$L_x \times L_y$$ square lattice Heisenberg antiferromagnet with $$L_x, L_y$$ odd and open boundary conditions, and for an $$L \times L$$ square lattice Heisenberg antiferromagnet with periodic boundary conditions and $$L$$ even, but with one site missing. We first compare with exact diagonalization the results for (i) an $$L_x = 3, L_y = 5$$ open boundary condition system, (ii) and an $$L = 4$$ period boundary condition system having one site missing. In figure 4, we show the dependence of the estimators for the ground state energy, and $$S_z(\pi, \pi)$$ as a function of the projection power $$m$$ in both of these cases. Also shown in figure 5 is a corresponding study of the performance of the original singlet sector algorithm for an $$L = 4$$ periodic boundary condition system. From these comparisons, it is clear that the performance of the modified algorithm is comparable to the performance of the original algorithm in the singlet sector, and thus our modification provides a viable method for studying antiferromagnets forced to have an $$S_{\text{tot}} = 1/2$$ ground state due to the nature of the finite sample.

In collaboration with Alet, we have used the method developed here to study the physics of continuous quantum phase transitions between Néel ordered antiferromagnets and valence-bond solid ordered quantum paramagnets in square lattice antiferromagnets with certain multispin interactions. The results of this study will appear separately in a future publication [11].
Here, we content ourselves with some illustrative physics results. Using our method, we can directly calculate $\langle S_z(\vec{r}) \rangle$ in the $S_{\text{tot}}^z = 1/2$, $S_{\text{tot}} = 1/2$ ground state of an $L \times L$ square lattice $S = 1/2$ Heisenberg antiferromagnet with open boundaries and odd $L$. In
Figure 5. Variation of the Monte Carlo estimates of the energy and $\langle m_s^2 \rangle$, the ground state expectation value of the square of the antiferromagnetic order parameter, of the 2D $S = 1/2$ Heisenberg antiferromagnet, normalized by their exact values obtained from exact diagonalization, plotted as a function of the projection length $2m$ normalized by the system volume $L^2 = L_xL_y$, for a $4 \times 4$ periodic system.

As noted by Metlitski and Sachdev [13], the effect of the open boundary condition is to decrease the sublattice magnetization near the boundary. This is then restored to its bulk value away from the boundary in a power-law manner [12, 13]. As demonstrated by [13], this boundary induced suppression goes away as a power law $1/|\vec{r}|$ at distance $|\vec{r}|$ from the edge.

On general grounds, one expects that $(-1)^\vec{r}\langle S^z(\vec{r}) \rangle$ will also obey this prediction of Metlitski and Sachdev, as would $\langle S^z(\vec{r}) \rangle$ on just the A-sublattice sites of the system, although these quantities are not directly related to the usual definition of the Néel order parameter (here $(-1)^\vec{r}$ equals +1 on an A-sublattice site and −1 on a B-sublattice site). With this in mind, we compare our results with the predictions from [13], and find extremely good agreement (figure 6 main panel), both with the predictions of [13] and the recent quantum Monte Carlo results for closely related quantities reported in the thesis of Hoglund [14], pointing to the usefulness of our approach.

Finally, we note that Wang and Sandvik [15] have recently used related ideas to develop a method for accessing $S_{\text{tot}} = 1$ and higher integer total spin states of antiferromagnetic clusters with an even number of sites but with an imbalance between

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Figure 6. Main panel: ground state spin texture \( \langle S^z(\vec{r}) \rangle \) in the \( S_{\text{tot}} = 1/2 \), \( S_{\text{tot}} = 1/2 \) ground state of \( L \times L \) spin-half Heisenberg antiferromagnets with \( L \) odd. This spin texture decays as \( \sim 1/x \) to the bulk value at distance \( x \) away from the boundary on all A-sublattice sites along a \( y \approx L/2 \) cut perpendicular to the boundary for \( L = 65, 81, \) and 101. Inset: \( \langle S^z(\vec{r}) \rangle \) on the A-sublattice sites along a diagonal and an edge of an \( 81 \times 81 \) system.

the numbers of A-sublattice and B-sublattice sites. Preliminary work suggests that it is feasible to combine these ideas with the ideas developed here in order to generalize our work and thereby access \( S_{\text{tot}} = 3/2 \) and higher half-integer total spin states of antiferromagnetic clusters with an odd number of sites.

A different kind of generalization also seems possible: a generalization of the original singlet sector algorithm has been used by Beach et al [16] and by Lou et al [17] to study \( SU(N) \) singlet ground states of bipartite \( SU(N) \) antiferromagnets in which the number of sites carrying the fundamental representation \( N \) equals the number of sites carrying the complex conjugate \( N^* \) of the fundamental representation. Preliminary investigation suggests that the ideas developed here can be generalized to this case as well, making it possible to also study \( SU(N) \) antiferromagnets with an odd number of sites, in which the number of sites carrying \( N \) is 1 more (or less) than the number of sites carrying \( N^* \). This will be explored in more detail in collaboration with Alet in a forthcoming publication and used to study the physics of non-magnetic impurities (vacancies) in \( SU(N) \) magnets [18].

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