Ground State Projection of Quantum Spin Systems in the Valence-Bond Basis

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A Monte Carlo method for quantum spin systems is formulated in the valence-bond basis. The nonorthogonality allows for an efficient importance-sampled projection of the ground state out of an arbitrary state. The method provides access to resonating valence-bond physics, enables a direct estimator for the singlet-triplet gap, and extends the class of models that can be studied without negative-sign problems. As a demonstration, the valence-bond distribution in the ground state of the 2D Heisenberg antiferromagnet is calculated. Generalizations of the method to fermion systems are also discussed.

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Quantum spin systems play a prominent role in current condensed matter research. Although much progress has been made in recent years, there are still formidable challenges remaining in exploring the plethora of possible ground states and excitations [1]. Gaining deeper understanding of quantum spin physics is not only important in the context of particular magnetic systems, but it could also give insights of broader relevance to correlated quantum matter, e.g., concerning quantum phase transitions [2,3].

Spin models such as the Heisenberg Hamiltonian, with interactions $J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j$, can be studied by a wide range of methods. Numerical finite-lattice calculations can, in principle, deliver results free of approximations, but, in practice, available computational methods are restricted to certain classes of models. For instance, density matrix renormalization [4] is essentially limited to one dimension and quantum Monte Carlo (QMC) techniques [5,6] can be used on a large scale only when the interactions are nonfrustrated. Even then, there are still often challenges in going to a lattice sufficiently large for reliable extrapolation to the infinite lattice. Developing more general and efficient computational methods, for frustrated as well as nonfrustrated systems, therefore continues to be an important field of research.

In this Letter, a QMC method for $S = 1/2$ Heisenberg models is presented which offers several advantages relative to state of the art ground state simulations (taking $T \to 0$ in world-line [5] or stochastic series expansion (SSE) [6] QMC with loop-cluster updates). The method is formulated in an overcomplete and nonorthogonal basis, which in the simplest case is the valence-bond (VB) basis, in which pairs of spins form singlets [7–10]. Any singlet state can be expanded in this basis, and the ground state can be projected out of an arbitrary VB state by applying a high power of the Hamiltonian H. Such a scheme was used by Liang [11], who started from a good trial wave function $|\Psi\rangle$ and improved it by sampling [12] terms of $(-H)^n|\Psi\rangle$, with a final extrapolation $n \to \infty$. Santoro *et al.* used the VB basis in a Green's function method [13]. There has been no follow-up on these pioneering works—the full potential of QMC in the VB basis has apparently not been realized. Here it will be shown how the nonorthogonality enables a fast importance-sampled projection without variational states or extrapolations. Triplet states can also be studied, and unpaired spins (spinons) can be introduced as well. There is, thus, direct access to degrees of freedom that are normally not available with QMC calculations but are of great theoretical interest. The valence bonds and spinons are the actors in resonating valence-bond physics [9], which is often used as a starting point for simplified quantum-dimer models [14] and field theories [2,3,15]. The method should, thus, facilitate closer contact with modern analytical treatments. Moreover, the method extends the range of models that can be studied without negative-sign problems.

Projection of a singlet state is here considered first, and then the scheme is extended to a triplet. As an illustration of results that can be obtained, the distribution of VB lengths in the ground state of the 2D Heisenberg model is presented. Finally, generalizations to a wider range of models in other related overcomplete bases are discussed.

The expansion in terms of VB states of a singlet ground state of N spins ($N/2$ valence bonds) is written as

$$|0\rangle = \sum_k f_k |(a_1^k, b_1^k) \cdots (a_{N/2}^k, b_{N/2}^k)\rangle = \sum_k f_k |S_k\rangle, \quad (1)$$

where (a_i^k, b_i^k) denotes two spins paired up in a singlet,

$$(a, b) = (\uparrow_a\downarrow_b - \downarrow_a\uparrow_b)/\sqrt{2}, \quad (2)$$

i.e., a valence bond, and k labels all bond tilings of the lattice (allowing arbitrary bond lengths). The notation $|S_k\rangle$ has been introduced for convenience. The expansion can always be made positive definite; any negative f_k can be made positive by switching the indices of one singlet.

Since the VB basis is overcomplete, the expansion coefficients are not unique, in general. However, the expansion of any state $|\Psi\rangle$ written in the VB basis of course has a unique expansion in energy eigenstates $|n\rangle$;

$$|\Psi\rangle = \sum_k g_k |S_k\rangle = \sum_n c_n |n\rangle. \quad (3)$$

Therefore, acting on this state with a high power ($n \to \infty$)

of the Hamiltonian projects out the ground state:

$$[-(H-C)]^n|\Psi\rangle = \sum_k g_{n,k}|S_k\rangle \rightarrow c_0|E_0 - C|^n|0\rangle. \quad (4)$$

A constant C has been subtracted to ensure that the ground state energy is the largest in magnitude. QMC methods based on (4) in the standard basis of eigenstates of all S_i^z are commonly used [16,17], although for bipartite systems they tend to be less efficient than low-temperature simulations with advanced finite-T methods [5,6]. However, for frustrated systems [17] and t-J models [18], where there are sign problems (nonpositive-definite $g_{n,k}$ and analogous mixed signs in other methods) projector methods are superior if a good trial state $|\Psi\rangle$ can be used.

The first observation underlying the projector method in the VB basis is that the application of a Heisenberg interaction operator on a VB state leads to a very simple rearrangement of valence bonds [8,11]. Consider the Heisenberg Hamiltonian, on any lattice, written as

$$H = -\sum_{\langle i,j\rangle} J_{ij}H_{ij}, \qquad H_{ij} = -\left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}\right). \quad (5)$$

Acting with H_{ab} on a VB state in which sites a and b belong to the same valence bond gives an eigenvalue of unity; $H_{ab}|\ldots(a,b)\ldots\rangle = |\ldots(a,b)\ldots\rangle$. Acting on sites belonging to different valence bonds gives a new basis state;

$$H_{bc}|\ldots(a,b)\ldots(c,d)\ldots\rangle = \tfrac{1}{2}|\ldots(a,d)\ldots(c,b)\ldots\rangle. \quad (6)$$

This *bond flip* is illustrated in Fig. 1. Here the sign is always positive when the indices are in the order indicated. This implies that a positive-definite representation of the projection $(-H)^n|\Psi\rangle$ can be achieved for a bipartite lattice, by defining (a,b) so that a is on sublattice A and b on sublattice B, as illustrated with arrows in Fig. 2. The convention also implies a positive-definite (1) [10].

For a nonfrustrated interaction, one can show that the projected ground state (4) contains only bonds connecting spins on different sublattices (bipartite bonds). Consider the VB configuration shown to the left in Fig. 1(b). With sites a, c in sublattice A and b, d in B, both the bonds are nonbipartite. When the operator has acted, the new bonds are bipartite. With a bipartite interaction, one cannot accomplish the reverse process (note that the Hamiltonian is not manifestly Hermitian in the VB basis), and, thus, if the trial state $|\Psi\rangle$ contains nonbipartite bonds, they will vanish after H has acted a number of times and cannot reappear. The ground state, hence, must contain only bipartite bonds.

For a frustrated interaction, nonbipartite bonds are generated and the flip (6) can lead to a minus sign [19]. It may also, in practice, not be possible to find a convention which renders all the expansion coefficients in (1) positive. The projection scheme still also works, in principle, for frustrated systems, as long as any negative signs are taken into account in the standard way [20].

With the Hamiltonian (5), $C = 0$ can be used in (4). To expand H^n, an index sequence $P_n = [a_1, b_1], \ldots, [a_n, b_n]$ is used to refer to an operator product $\prod_p H_{a_p b_p}$. One of the VB basis states can be chosen as the trial state; $|\Psi\rangle = |S_0\rangle$ [21]. The projected state is then

$$(-H)^n|S_0\rangle = \sum_{P_n}\prod_{p=1}^{n} J_{a_p b_p}H_{a_p b_p}|S_0\rangle = \sum_{P_n} W(P_n)|S(P_n)\rangle, \quad (7)$$

where $|S(P_n)\rangle$ denotes the (normalized) state obtained when the operators have acted on $|S_0\rangle$ and $W(P_n) = \prod_p w_{a_p b_p}$. The factors w_{ab} are $\frac{1}{2}J_{ab}$ or J_{ab} for operations with H_{ab} that cause bond flips and are diagonal, respectively, in the course of propagating the state from $|S_0\rangle$ to $|S(P_n)\rangle$. Note that no operator H_{ab} can destroy the state in (7), i.e., all $W(P_n) \neq 0$. This will be taken advantage of in constructing an importance-sampling scheme that would not be possible in the z basis, where there are enormous constraints on the operator products.

To calculate the ground state energy, the overlap with an arbitrary reference state $|R\rangle$ can be taken;

$$E_0 = \frac{\langle R|H|0\rangle}{\langle R|0\rangle} = \frac{\sum_{P_n} W(P_n)\langle R|H|S(P_n)\rangle}{\sum_{P_n} W(P_n)\langle R|S(P_n)\rangle}. \quad (8)$$

One can always choose a state with equal overlap with all basis states, and, hence, all $\langle R|S\rangle$ overlaps cancel. If P_n is sampled with probability $\propto |W(P_n)|$, the energy is

$$E_0 = -\frac{1}{\langle s\rangle}\sum_{\langle i,j\rangle} J_{ij}\left\langle s\left(n_{ij} + \frac{1}{2}(1-n_{ij})q_{ij}\right)\right\rangle, \quad (9)$$

where $n_{ij} = 1$ (0) if there is (is not) a bond connecting sites i and j in $|S(P_n)\rangle$. For a frustrated system, $s = \pm 1$ is the product of phase factors ± 1 arising when propagating $|S_0\rangle$ to $|S(P_n)\rangle$ with the string P_n, and $q_{ij} = \pm 1$ arises when H_{ij}

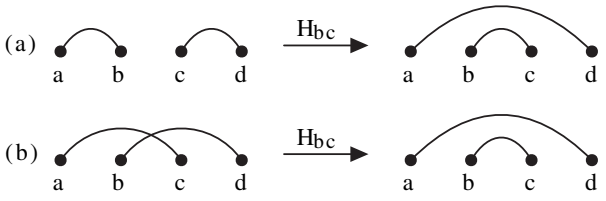

FIG. 1. Action of a bond operator on two VB states.

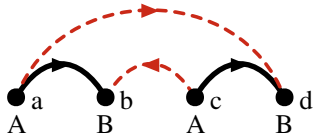

FIG. 2 (color online). Singlet convention for a system with sublattices A and B. The arrows indicate the order of the spins in the singlets, e.g., $c \rightarrow b$ means $(c,b) = (\uparrow_c\downarrow_b - \downarrow_c\uparrow_b)/\sqrt{2}$.

is applied once more. For a bipartite system, $s = q_{ij} = 1$ and, thus, $E_0 = -\frac{1}{2}\sum_{ij} J_{ij}\langle n_{ij} + 1\rangle$.

An expectation value $\langle A\rangle = \langle 0|A|0\rangle/\langle 0|0\rangle$ of an arbitrary operator can be written in terms of two projected states, obtained from the same trial state $|S_0\rangle$ propagated with two different operator strings P_n and Q_n;

$$\langle A\rangle = \frac{\sum_{P_n}\sum_{Q_n} W(P_n)W(Q_n)\langle S(Q_n)|A|S(P_n)\rangle}{\sum_{P_n}\sum_{Q_n} W(P_n)W(Q_n)\langle S(Q_n)|S(P_n)\rangle}. \quad (10)$$

The weight function to be used in importance sampling is thus $W(P_n)W(Q_n)\langle S(Q_n)|S(P_n)\rangle$, and the operator estimator is $\langle S(Q_n)|A|S(P_n)\rangle/\langle S(Q_n)|S(P_n)\rangle$.

For a bipartite system, the overlap of two VB states is determined by the loops formed when the bonds are superimposed [22], as illustrated in Fig. 3 (with frustration, a sign has to be determined as well). Matrix elements $\langle S_\alpha|\mathbf{S}_i\cdot\mathbf{S}_j|S_\beta\rangle$ are also easily obtained from these loops; $\langle S_\alpha|\mathbf{S}_i\cdot\mathbf{S}_j|S_\beta\rangle/\langle S_\alpha|S_\beta\rangle = \pm 3/4$ if sites i and j belong to the same loop ($+$ and $-$ for i, j on the same and different sublattices, respectively, in the case of a bipartite lattice), and 0 otherwise.

A remarkable aspect of the VB basis is that Eqs. (8) and (10) can be efficiently sampled in an almost trivial way, in steps where a few (r) of the operators in the product P_n are changed at random. Naively, one might expect that the acceptance rate should become very low for large expansion order n, but this turns out not to be the case. With $r = 4$, the acceptance rate in the case of the 2D Heisenberg model is $\approx 40\%$, almost independently of n and the lattice size. The new weight can be computed by performing the full propagation of the state $|S_0\rangle$ with the updated product(s) in (7) [and calculating the new overlap in the case of (10)]. Recalculating the full weight, instead of just a ratio, may seem like an inefficient proposition. However, if n has to be increased with the system size as N^α in order to converge to the ground state, $N^{2\alpha}$ operations [$N^{1+\alpha}$ if $\alpha < 1$ in the case of (10)] are needed to update the full operator sequence (attempting n/r updates of r operators is defined as one sweep; several measurements are carried out during each sweep). In $T \to 0$ calculations with finite-T methods [5,6], the scaling is $N^{1+\alpha'}$ if $T \propto N^{-\alpha'}$. Hence, if $\alpha, \alpha' \approx 1$ the scaling is very similar. The gap to the lowest singlet excitation dictates α, and, hence, in many cases $\alpha < 1$ suffices. An even faster sampling could likely be achieved by using a linked operator list [6]; such an improvement will be left for future work.

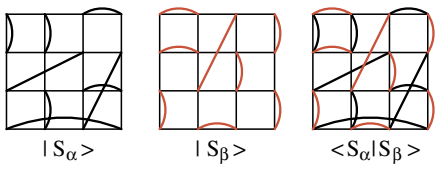

FIG. 3 (color online). Two VB states in two dimensions and their overlap in terms of loops formed by superimposing the two bond configurations. In this case, there are $N_v = 8$ valence bonds and $N_l = 3$ loops, and $\langle S_\alpha|S_\beta\rangle = 2^{N_l - N_v} = 1/32$ [22].

In order to study a triplet state, consider a triplet bond; $[a, b]_0 = (\uparrow_a\downarrow_b + \downarrow_a\uparrow_b)/\sqrt{2}$. The eigenvalue of H_{ab} operating on $[a, b]_0$ is 0. If H_{bc} is applied to $[a, b]_0(c, d)$, the reconfiguration of the bonds is exactly as in (6); the new state is $[a, d]_0(c, b)/2$. Hence, if there is no diagonal operation on the triplet, the triplet bond (if there is only one) behaves exactly as a singlet, and the only change in the scheme is in the operator estimators. This enables an improved estimator for, e.g., the singlet-triplet gap: Carrying out the simulation with only singlets, one of the bonds can be flagged as a triplet at the measurement stage. The E_1 estimator can be averaged over all $N/2$ initial triplet choices, with contributions coming only from surviving configurations, i.e., those for which there are no diagonal operations on the triplet (the survival ratio depends on n). This does not change the scaling $N^{2\alpha}$ of the simulation and can vastly improve the estimate of the gap compared to $E_1 - E_0$ obtained from two independent simulations (the improvement is due largely to partial cancellation of correlated statistical errors in E_0 and E_1). For example, for the 2D Heisenberg model with $N = 64 \times 64$, a projection with $n = 15N$ and 10^6 updating sweeps gave $E_0/N = 0.669\,449(2)$ and the finite-size gap $E_1 - E_0 = 0.0041(2)$, corresponding to an accuracy gain of 60 times for the gap, or a CPU-time reduction of 7000. The energy agrees with that obtained using the SSE method [6]; $E_0/N = 0.669\,450(1)$, confirming the unbiased nature of both calculations.

It is important to verify that the method works for frustrated interactions as well, although the basic formulation discussed here [19] is not likely to be practically useful for large frustrated lattices. The method should, however, be applicable to models with local sign problems, e.g., lattices with frustrated impurities. Checks against exact diagonalization results confirm that the scheme indeed works. For a 4×4 system with nearest- and next-nearest-neighbor interactions J_1 and J_2, at $J_2/J_1 = 0.1$ a ground state energy $E_0/N = 0.659\,86(4)$ was obtained using $n = 3N$ and $|S_0\rangle$ a columnar dimer state (5×10^9 updating sweeps), which matches well the exact $E_0/N = 0.659\,817$. The average sign in this case is $\langle s\rangle \approx 0.074$.

As an application of the method, the VB length distribution in the ground state of the 2D Heisenberg model is presented next. Liang, Doucot, and Anderson [10] studied variational wave functions with VB state amplitudes $f_k = \prod_i h(a_i^k, b_i^k)$ in Eq. (1). For $h \propto 1/r^p$, where r is the bond length, they concluded that there is long-range Néel order for $p < 5$. The best variational energy was obtained with $p = 4$, but the dependence on p for $2 \le p \le 5$ was quite weak. The bond amplitude $h(x, y)$ does not correspond exactly to the probability $P(x, y) \propto \sum_k f_k n_{xy}^k$ [where n_{xy}^k is the number of length-(x, y) bonds in VB state k], but simulations of the type used in Ref. [10] confirm that, if

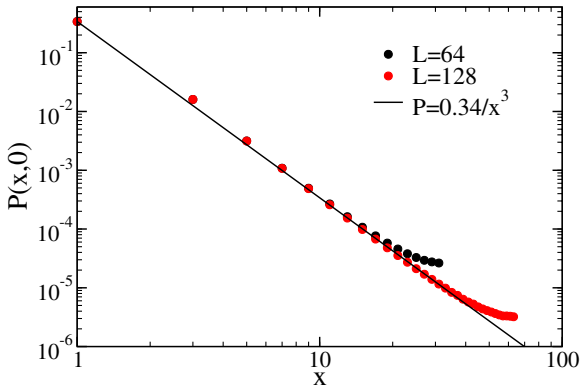

FIG. 4 (color online). The bond-length probability for bonds along the line $(x, 0)$ in the 2D Heisenberg ground state wave function.

$h(r) \propto 1/r^p$, then also $P(r) \propto 1/r^p$. Note also that $P(x, y)$ is not a ground state expectation value but a property of the wave function coefficients [but $\langle 0|n_{xy}|0\rangle$ turns out to be almost identical to $P(x, y)$]. A potential worry is that, since the VB basis is overcomplete, the bond distribution is not unique. However, the way the projection is done corresponds to a uniform averaging over all possible VB ground state wave functions; $P(x, y)$ defined this way clearly has a well-defined meaning.

Calculations were carried out on periodic $L \times L$ lattices with $L = 64$ and 128, with n up to $15N$ and $20N$, respectively (convergence was checked). The results shown in Fig. 4 suggest that $P(r) \sim 1/r^3$ (there is no notable angular dependence). It would be interesting to understand this result from an analytical starting point and also to study the probability distribution for a quantum-critical system, e.g., the Heisenberg bilayer [23].

The VB projector scheme opens up a range of interesting avenues to be explored. The VB (+triplets) basis is formed out of the 2-site eigenstates of $\mathbf{S}_i \cdot \mathbf{S}_j$ and, hence, is particularly suitable for Heisenberg models. The method can also be extended, without sign problems, to higher-order (nonfrustrating) interactions of the form $-(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}) \times (\mathbf{S}_k \cdot \mathbf{S}_l - \frac{1}{4})$. This interaction has a sign problem in the z basis, and, hence, the present method solves a class of sign problems. Although there are sign problems for frustrated systems in general, the VB basis opens opportunities to explore cancellation schemes based on overcompleteness [19]. Good sign-problem-free approximations could also perhaps be developed.

It is possible to generalize the VB basis to other Hilbert spaces, with different types of bonds corresponding to eigenstates of the Hamiltonian on two sites (or even >2 sites, although the complexity of the approach then increases considerably). Such schemes for t-J and Hubbard models will be investigated. Although there will clearly be sign problems for fermions, a generalized bond-state basis also offers opportunities for new variational wave functions, which could be further refined with the projector method. Access to the VB (and generalized) degrees of freedom also enables construction of interesting Hamiltonians acting on bonds. Such studies could clarify the relationships between quantum-dimer [14] and spin models. Studying the properties (such as the length distribution) of a triplet bond in the "singlet soup" of a gapped or critical system gives information pertaining to the nature of the spinon bound state (magnon) or spinon doconfinement. This should be very useful, e.g., in studies of deconfined quantum criticality [3,15].

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