Sign rules for anisotropic quantum spin systems

R. F. Bishop, D. J. J. Farnell, and J. B. Parkinson

Department of Physics, University of Manchester Institute of Science and Technology (UMIST), P. O. Box 88, Manchester M60 1QD, United Kingdom

(Received 23 August 1999; revised manuscript received 19 November 1999)

We present exact “sign rules” for various spin- s anisotropic spin-lattice models. It is shown that, after a simple transformation which utilizes these sign rules, the ground-state wave function of the transformed Hamiltonian is positive definite. Using these results exact statements for various expectation values of off-diagonal operators are presented, and transitions in the behavior of these expectation values are observed at particular values of the anisotropy. Furthermore, the importance of such sign rules in variational calculations and quantum Monte Carlo calculations is emphasized. This is illustrated by a simple variational treatment of a one-dimensional anisotropic spin model.

Exact results for quantum many-body systems are rare. They are therefore always valuable as yardsticks against which numerical or semianalytical methods may be measured. Such exact results acquire additional value when they can be used as actual input to improve one or more of the approximate methods. Such input is often useful, for example, in tailoring a trial or starting many-body wave function to preserve certain exact properties. In some instances they can even be practically essential for the successful implementation of particular techniques. An example is provided by the fixed-node quantum Monte Carlo (QMC) method, which provides a means to circumvent the infamous “minus sign problem” inherent in simulating many-fermion systems, but at the cost of requiring good (and, ideally, exact) information on the nodal surface of the many-fermion wave function. In this paper we provide several exact results of such “sign rules” (which exactly define the nodal surfaces) for some general classes of anisotropic spin-lattice models. These models are of considerable interest both in their own right and as models of real (low-dimensional) magnetic materials.

In 1955 Marshall¹ used a variational method to study the isotropic spin-half Heisenberg antiferromagnet (HAF) specified by the Hamiltonian

$$H = J \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j, \quad (1)$$

where the sum on $\langle i,j \rangle$ counts each nearest-neighbor pair once and once only on the lattice on which Eq. (1) is specified, and J is positive. Furthermore, the lattice was assumed to be *bipartite* (i.e., the lattice can be divided into two sublattices (A, B) such that all nearest neighbors of a site on one sublattice lie on the other and *vice versa*). The total number of atoms was N and the spatial dimensionality was not restricted. In the course of this paper it was proven that the exact ground-state wave function can be written as

$$|\Psi\rangle = \sum_I c_I |I\rangle, \quad (2)$$

where $\{|I\rangle\}$ are the usual basis states in the z -aligned Ising representation, specified by the tensor products of eigenstates of the Pauli operator $\sigma_i^z \equiv 2s_i^z$ with eigenvalues ± 1 , at all sites i . The coefficients $\{c_I\}$ were proven to have the property that

$$c_I = (-1)^{\phi(I)} a_I, \quad (3)$$

where the coefficients $\{a_I\}$ are all positive real numbers or zero and $\phi(I)$ is the eigenvalue, with respect to the corresponding eigenstate $|I\rangle$, of the operator

$$\phi = n_A, \quad (4)$$

which counts all of the spin-half “up” states on the A sublattice. Lieb and Mattis² were able to prove that the ground state of the HAF was a singlet following the work of Marshall¹ and Lieb, Schultz, and Mattis.³

Indeed, these results for the HAF model on a bipartite lattice are a consequence of a property of nonpositive matrices. The Hamiltonian of Eq. (1) is transformed in the following manner:

$$H' = e^{i\pi\phi} H e^{-i\pi\phi}. \quad (5)$$

It is seen that H' of Eq. (5) now contains only nonpositive off-diagonal interactions with respect to the Ising basis states. Hence the ground state of the HAF corresponds to the eigenstate of largest magnitude eigenvalue which is positive definite via the Perron–Frobenius theorem.⁴ Munro⁵ and Parkinson⁶ were also able to extend these results to the spin-one biquadratic model on a bipartite lattice in various phases. They showed that the ground eigenstates are positive definite and also nondegenerate. Finally, Klein⁷ utilized this knowledge afforded by the Perron–Frobenius theorem for Heisenberg models to prove six theorems relating to ground-state features of these models. Among these theorems was one which stated that the ground-state expectation value of the operator $\mathbf{s}_i \cdot \mathbf{s}_j$ for these models is positive or negative depending on whether i and j are on the same or different sublattices, respectively.

The usefulness of sign rules in numerical and analytical calculations of lattice quantum spin systems has also previously been observed, for example, by Pati⁸ for the alternating

spin-1/spin-1/2 chain. Their utility in variational calculations, such as those employing a Jastrow Ansatz for the trial wave function, has been demonstrated many times. Such trial wave functions constructed on the basis of sign rules have been considered, for example, by Retzlaff, Richter, and Ivanov.⁹ We note that sign rules, such as those presented here, have also been seen to accelerate density matrix renormalization-group (DMRG) calculations¹⁰ by up to an order of magnitude. Finally, we note that the presence of such sign rules can also present an excellent check of approximate *ab initio* calculations. This has been observed, for example, in approximate coupled cluster method (CCM) calculations^{11,12} for various lattice quantum spin systems.

In this article we present sign rules for various spin- s anisotropic spin systems. The transformation of Eq. (5) for these sign rules is utilized to force the off-diagonal interactions of the Hamiltonians to be always nonpositive. A property of positive or negative semi-definite matrices is that the eigenvector corresponding to the eigenvalue of H' of largest magnitude (i.e., the ground-state energy here) contains only non-negative elements, and so the ground-state wave function is positive definite.

The first model that we consider is the XYZ model, which has a Hamiltonian given by

$$\begin{aligned} H_{XYZ} &\equiv \sum_{[i,j]} \{J_{i,j}^x s_i^x s_j^x + J_{i,j}^y s_i^y s_j^y + J_{i,j}^z s_i^z s_j^z\} \\ &= \sum_{[i,j]} \{a_{i,j} s_i^z s_j^z + b_{i,j} (s_i^+ s_j^- + s_i^- s_j^+) \\ &\quad + c_{i,j} (s_i^+ s_j^+ + s_i^- s_j^-)\}, \end{aligned} \quad (6)$$

where $\{s_i^a; a=x,y,z\}$ are the usual spin operators, in terms of which $s_i^\pm \equiv s_i^x \pm i s_i^y$, and where $a_{i,j} \equiv J_{i,j}^z$, $b_{i,j} \equiv (J_{i,j}^x + J_{i,j}^y)/4$ and $c \equiv (J_{i,j}^x - J_{i,j}^y)/4$. The index i in Eq. (6) runs over all N sites on a bipartite lattice and j runs over all sites which are on the opposite sublattice to i . The square bracket $[i,j]$ indicates that each bond is counted once and once only.

The second such model that we shall consider is the single-ion anisotropy (SIA) model, given by

$$\begin{aligned} H_{SIA} &\equiv D \sum_i (s_i^x)^2 + \sum_{[i,j]} J_{i,j} \mathbf{s}_i \cdot \mathbf{s}_j \\ &= \sum_{[i,j]} J_{i,j} \left\{ s_i^z s_j^z + \frac{1}{2} (s_i^+ s_j^- + s_i^- s_j^+) \right\} \\ &\quad + \frac{D}{4} \sum_i \{ (s_i^+)^2 + (s_i^-)^2 + 2[s(s+1) - (s_i^z)^2] \}. \end{aligned} \quad (7)$$

Again, the index i in Eq. (7) runs over all N sites on a bipartite lattice and j runs over all sites which are on the opposite sublattice to i .

Finally, we also consider the transverse Ising model (TIM), which has a Hamiltonian given by

$$H_{TIM} \equiv \sum_{[k_1, k_2]} \Omega_{k_1, k_2} s_{k_1}^z s_{k_2}^z + \lambda \sum_i s_i^x$$

$$= \sum_{[k_1, k_2]} \Omega_{k_1, k_2} s_{k_1}^z s_{k_2}^z + \frac{\lambda}{2} \sum_i (s_i^+ + s_i^-). \quad (8)$$

For the TIM, we place no restriction on the lattice type, and k_1 and k_2 are allowed to run over all lattice sites with $k_1 \neq k_2$. Furthermore, we note that adding extra terms to the Hamiltonians in Eqs. (6)–(8) which are diagonal in the z -aligned Ising basis (such as an external magnetic field or crystal field anisotropy in the z direction), or letting i and j in Eqs. (6) and (7) run over the same sublattice but, in this case, explicitly restricting $b_{i,j} \leq 0$ in Eq. (6) and $J_{i,j} \leq 0$ in Eq. (7), do not change the following sign rules.

We now define the following operators:

$$m_A \equiv \sum_{l_A} s_{l_A}^z; \quad m \equiv \sum_l s_l^z, \quad (9)$$

where l_A runs over all $N/2$ A -sublattice sites and l runs over all N sites on both sublattices. Note that for eigenstate $|I\rangle = \otimes_{l=1}^N |s_l, m_l\rangle$ (where $s_l^z |s_l, m_l\rangle = m_l |s_l, m_l\rangle$ with $m_l = -s_l, -s_l+1, \dots, s_l-1, s_l$), m and m_A have eigenvalues denoted by $m(I)$ and $m_A(I)$, respectively. Note that the following sign rules are fully defined by the form of the operator ϕ which, in turn, gives the set of eigenvalues $\{\phi(I)\}$. Furthermore, these eigenvalues determine the relative signs of the $\{c_I\}$ coefficients via Eq. (3) for the expansion of the ground-state wave functions, Eq. (2), of the anisotropic Hamiltonians of Eqs. (6)–(8). The sign rules are thus defined by

$$\begin{aligned} \phi &= 1; & \text{rule (A)} \\ \phi &= m_A; & \text{rule (B)} \\ \phi &= m/2; & \text{rule (C)} \\ \phi &= m_A + m/2; & \text{rule (D)} \\ \phi &= m; & \text{rule (E)}. \end{aligned} \quad (10)$$

Furthermore, note that rule (B) is a reformulation, for general spin quantum number, of the Marshall-Peierls sign rule for the spin-half HAF given by Eqs. (3) and (4). It is readily found that the first four sign rules apply to the XYZ and SIA models in the following regimes:

Rule	XYZ model	SIA model
(A)	$b_{i,j} \leq 0, c_{i,j} \leq 0$	$D \leq 0, J_{i,j} \leq 0$
(B)	$b_{i,j} > 0, c_{i,j} \geq 0$	$D \leq 0, J_{i,j} > 0$
(C)	$b_{i,j} \leq 0, c_{i,j} > 0$	$D > 0, J_{i,j} \leq 0$
(D)	$b_{i,j} > 0, c_{i,j} < 0$	$D > 0, J_{i,j} > 0$

(11)

for all values of i and j on opposite sublattices. [Note again that we do not allow the existence of any “frustrated” interactions in Eqs. (6) or (7).] For the TIM, it is found that rule (A) applies when $\lambda \leq 0$, and rule (E) applies when $\lambda > 0$ for all signs and strengths of the coefficients Ω_{k_1, k_2} of the Ising interaction in Eq. (8).

We once again note that the off-diagonal interactions of H' of Eq. (5) with respect to a complete set of z -aligned Ising states are now always nonpositive, such that

$$\langle I_1 | (H' - w) | I_2 \rangle \leq 0, \quad \forall \quad I_1, I_2, \quad (12)$$

where w is a positive number large enough to force all of the diagonal elements to be negative. Hence the proof of the sign rules is now manifest because the matrix elements of Eq. (12) are nonpositive for all z -aligned Ising states I_1 and I_2 . The theory of nonpositive matrices now states that the eigenvector corresponding to the eigenvalue of *lowest* value must be positive definite, and the interested reader is referred to Ref. 4 for more information regarding this property. Hence the ground-state eigenvector of $(H' - w)$, and therefore also H' , contains only non-negative elements and so is written as $|\Psi'\rangle = \sum_I a_I |I\rangle$, where $a_I \geq 0 \forall I$. In addition, the ground-state eigenvector of H may now be written as $|\Psi\rangle = \sum_I \exp[-i\pi\phi(I)] a_I |I\rangle$, where $a_I \geq 0 \forall I$. We note that in all cases, although the individual phase factors $\exp[-i\pi\phi(I)]$ may be complex, the relative phase factors are always real in the specified regimes. The following inequality,

$$\langle I_1 | G | I_2 \rangle \geq 0 \quad \forall \quad I_1, I_2, \quad (13)$$

may also readily be proven for a variety of operators, $G = G[H]$, which depend on the Hamiltonian. Particularly important examples include $G = 1 + \alpha(H' - w)$, $G = [\alpha(H' - w)]^n$ (where n is a positive integer), or $G = \exp[\alpha(H' - w)]$, in which $\alpha < 0$ for these cases. Such relationships are of use in quantum Monte Carlo calculations at both zero and nonzero temperatures, as described in more detail below.

In the above treatment, no mention of *frustration* has been made. Classically, frustration implies that the classical (anti)ferromagnetic ground state is no longer the true ground state, and the spins cant at various angles such that the expectation values of the bonds between these spins have less than their saturated (anti)ferromagnetic values. [For example, the classical ground state of the J_1 - J_2 model on the linear chain, with both nearest-neighbor (J_1) and next-nearest-neighbor (J_2) interactions, in the frustrated regime is a "spiral" spin state.] However, from a quantum-mechanical viewpoint it is more difficult to know what these saturated values are, and even definitions of frustration in a quantum sense become more problematical. Indeed, with the addition of frustrating off-diagonal terms in H it is seen that it is much more difficult (if not often impossible) to prove a sign rule within an Ising basis, as it is difficult to determine a way in which every single off-diagonal "bond" can always give a negative energy contribution. By contrast this can always be achieved for the unfrustrated spin models considered in this article. However, one may, on the other hand, sometimes be able to circumvent this difficulty by utilizing a different (nonclassical) set of basis states. For example, a dimer basis was used for the spin-half J_1 - J_2 model for the linear chain¹³ in a frustrated region, (i.e., $0 < J_2/J_1 < 0.5$). As an alternative, one may also use approximate methods, such as the CCM,^{11,12} in order to probe the nodal surfaces of frustrated quantum spin models within the Ising basis.

It is also possible to prove exact relations⁷ (in some cases) for expectation values of various off-diagonal operators. In order to illustrate this we define an XXZ model for a bipartite lattice in which we set $J_{i,j}^x = J_{i,j}^y$ and $J_{i,j}^z = 1$ in Eq. (6). Hence we see from the table above that the sign rules are of type (A) for $J_{i,j}^x \leq 0$ and of type (B) for $J_{i,j}^x > 0$. We define the spin-spin correlation function in the x direction, given by

$$G^{xx}(r) = \frac{\langle \Psi | \sum_I s_I^x s_{I+r}^x | \Psi \rangle}{N \langle \Psi | \Psi \rangle}, \quad (14)$$

and the localized magnetization in the x direction to be

$$M^x(l) = \frac{\langle \Psi | s_l^x | \Psi \rangle}{\langle \Psi | \Psi \rangle}. \quad (15)$$

For the XXZ model with $J_{i,j}^x > 0$, it can be shown that if r in Eq. (14) connects sites on opposite sublattices then $G^{xx}(r) \leq 0$, while if r connects sites on the same sublattice then $G^{xx}(r) \geq 0$. Similarly for $J_{i,j}^x < 0$, it can be shown that the sign of $M^x(l)$ when l is a site on one particular sublattice must be the opposite to the sign of $M^x(l)$ when l is a site on the other sublattice. For $J_{i,j}^x < 0$, one can show that $G^{xx}(r) \geq 0 \forall r$, and that $M^x(l) \geq 0 \forall l$. For the transverse Ising model, it is found for any value of λ that $G^{xx}(r) \geq 0 \forall r$. By contrast, it is found that $M^x(l) \leq 0 \forall l$ for $\lambda > 0$, and that $M^x(l) \geq 0 \forall l$ for $\lambda < 0$. We note that other such relations exist for the models presented here, although they are not discussed further in this article.

In order to illustrate further the usefulness of the sign rules given here, we now also perform a simple variational calculation for a spin-half one-dimensional model in which the anisotropy is in the x direction such that $J_{i,j}^x \equiv -\Delta$, $J_{i,j}^y = 1$, and $J_{i,j}^z = -1$ in Eq. (6) and i and j are always nearest neighbors. Hence from Eq. (11) the sign rules are of type (A) for $\Delta \geq 1$, of type (D) for $-1 < \Delta < 1$, and of type (B) for $\Delta \leq -1$. The ground-state energy of this system using Eq. (2) may be written as

$$E = \frac{\sum_{I_1, I_2} c_{I_1}^* c_{I_2} \langle I_1 | H | I_2 \rangle}{\sum_{I'} |c_{I'}|^2}. \quad (16)$$

In order to treat this model variationally we now employ a Jastrow Ansatz, given by

$$c_I = (-1)^{\phi(I)} \langle I | \prod_{i < j} [1 + f(i, j)(P_i^\dagger P_j^\dagger + P_i^\dagger P_j)] | I \rangle, \quad (17)$$

where $P^\dagger$ and P are the usual projection operators onto the spin-half up and down states, respectively. The simplest approximation is to set the value of $f(i, j)$ to be f_1 (a scalar variable) if i and j are nearest neighbors, and to be zero otherwise. The expectation value of Eq. (16) may now be evaluated directly, although we explicitly restrict the sums over all states in Eq. (16) to those states in which $m(I)$ is an even number in order to reflect the symmetries of the Hamiltonian. The variational ground-state energy is minimized with respect to f_1 at each value of Δ , and the different sign rules for this system are utilized in separate calculations. We find that the best results for this variational Ansatz (for chains of length $N \leq 16$) are those which utilize the correct sign rule in each regime, and Fig. 1 illustrates these results compared to those of an exact diagonalization calculation for a chain of length $N = 12$. (The accuracy of the variational

FIG. 1. Results for the ground-state energy of an anisotropic spin-half quantum spin chain (described in the text) of length $N = 12$. The variational calculation utilizes the Jastrow ansatz of Eq. (17) in which the sign rules (A), (B), and (D) are used in separate calculations and these results are compared to those of an exact diagonalization of this system.

calculations with $N=12$ compared to extrapolation in the limit $N \rightarrow \infty$ via Padé approximants is estimated to be within about 4% for all Δ shown.)

This result is clearly true for any case in which one can prove an exact sign rule [e.g., those defined by Eqs. (3) and (10)] for a given model because any other choice would always contribute at least one nonzero positive contribution to the expectation energy from one of the off-diagonal contributions (i.e., $I_1 \neq I_2$) in Eq. (16). We may therefore infer that the best possible variational Ansatz for a given model must always utilize the correct sign rule in the correct regime. However, a direct evaluation of the sums in Eq. (16) scales exponentially with increasing lattice size N , and so one must evaluate these summations using Monte Carlo (MC) techniques. In order to explain how this is achieved, we define a *probability distribution* for the Ising states $\{|I\rangle\}$, given by

$$P(I) = \frac{|c_I|^2}{\sum_{I'} |c_{I'}|^2}, \quad (18)$$

and the *local energy* of these states, given by

$$E_L(I) = \sum_{I_1} \frac{c_{I_1}}{c_I} \langle I | H | I_1 \rangle. \quad (19)$$

Equation (16) may be equivalently written as

$$E = \sum_I P(I) E_L(I), \quad (20)$$

where the sums over I_1 in Eq. (19) and I in Eq. (20) run over all, or possibly some, symmetry-constrained subset [e.g., the subset of Ising basis states $|I\rangle$ for which $m(I)$ is even], of the full set of Ising basis states. The MC procedure approximates the summation over I by performing a directed random walk with respect to $|I\rangle$ based on the probability distribution $P(I)$. At each point of the MC “summation” procedure one “steps” from one state $|I\rangle$ to another $|I'\rangle$ (where $|I'\rangle$ is one of a number of states accessible to $|I\rangle$ via the off-diagonal elements of H) with a given probability which is dependent

on $P(I)$ and $P(I')$. Hence it is possible to “cover” all possible Ising states given enough run time, although one samples the most important states the most often. Hence in this manner an accurate approximation (to within statistical error) to the sum in Eq. (20) is built up. Also, the exponentially increasing problem with lattice size N is reduced to a problem that scales linearly with both N and the number of MC moves in a particular run. Hence systems of larger lattice size may be treated.

We note, however, that the sign rule *does not* affect the random walk which simulates the summation over $|I\rangle$ in Eq. (20) in such a variational MC calculation because the probability distribution of Eq. (18) is proportional to $|c_I|^2$. By contrast, we may see from the expression for the local energy of Eq. (19) that each and every off-diagonal contribution (i.e., $I \neq I_1$) to the local energy can only be ensured *always* to be negative when the correct sign rule in the correct regime is used. The average variational ground-state energy, evaluated using the MC procedure outlined above, is the average of the local energies throughout the lifetime of the run. Hence the average variational MC ground-state energy can only ever be ensured to be lowest (to within statistical error) when the correct sign rule is utilized within the variational Ansatz [e.g., in the Jastrow Ansatz of Eq. (17)].

Let us turn our attention from variational MC estimates to full stochastic simulations of finite lattices by QMC techniques. All QMC methods at zero temperature basically project the exact ground state $|\Psi\rangle$ of a given many-body Hamiltonian H out of an initial trial state $|\Phi\rangle$ not orthogonal to $|\Psi\rangle$, by repeated applications of some suitable projection operator, $G = G(H)$. This operation can be formally expressed as a path integral over many-particle trajectories in configuration space. Furthermore, it can thus be represented by a stochastic process, which may itself be simulated computationally by the random walks of a sampled set of independent “walkers” through the configuration space. The main limitation to the applicability of such QMC techniques arises from the positivity requirement,

$$p(c, c') \equiv \langle c | G | c' \rangle \frac{\Phi(c')}{\Phi(c)} > 0, \quad (21)$$

on the probability $p(c, c')$ for a walker to make a transition from an initial configuration $|c\rangle$ to another configuration $|c'\rangle$ along a random walk, where $\Phi(c)$ is the wave function of the initial trial state.

For fermionic systems, the minus sign problem associated with $p(c, c')$ ensures that QMC calculations are much more difficult than for bosons. Thus the computer time for bosonic simulations to give results of a specified accuracy scales algebraically with (i.e., as some positive power of) the system size N . By contrast, when the wave function being sampled is not positive definite, and hence cannot itself be regarded as a probability distribution, no “exact” simulation method has been discovered that does not scale exponentially with N . Without some prior knowledge of the nodal surface a QMC simulation will always eventually relax to the corresponding bosonic wave function. For the typical spin-lattice problem for which no such exact knowledge is available most QMC attempts to alleviate the minus sign problem, such as transient estimation, are infeasible due to its severity. In these

cases a recently proposed lattice variant¹⁴ of the fixed-node QMC (FNQMC) method¹⁵ seems to provide the only practicable QMC-based approach.

For the case of lattice quantum spin systems at zero temperature, if we now set the projection operator G to be defined by, for example, $G = \exp[\alpha(H' - w)]$ with $\alpha \leq 0$, and we also set $\Phi(c) \geq 0 \forall c$, then Eq. (13) implies that the positivity requirement of Eq. (21) is always satisfied. As the H' of Eq. (5) is a unitary similarity transformed version of the original Hamiltonian H , this implies that all of the eigenvalues remain the same for H' as for H . Furthermore, the subtraction of the positive constant w only produces a negative offset of strength $-w$ to every eigenvalue of H' (although this operation does not affect the eigenvectors at all). Hence it is seen that the presence of a sign rule completely circumvents the problem of maintaining the positivity requirement of Eq. (21). However, it is also noted that the local energy should not (significantly) fluctuate in sign for different Ising states, I , when the sign rules are utilized. This is because all of the off-diagonal contributions to the local energy always given a negative contribution, as observed for the variational calculations presented above. Hence the damaging effect of the

fluctuation of the signs of the expectation values, which lead to increasing statistical error with increasing simulation length, is also removed via the utilization of sign rules.

Generally, results of FNQMC calculations are exact, within statistical errors limited solely by available computing power, only when the nodal surfaces of both the trial and exact ground-state wave functions coincide. Otherwise they yield variational upper bounds for the energy. On the other hand, other ground-state quantities such as the (magnetization or) staggered magnetization may be poorly estimated even when the energy is well estimated. How errors in the nodal surface affect such quantities is not well understood. In principle, however, their effects can be large. In this context the importance of such sign rules as those presented here becomes clear, in that they permit a complete circumvention of the QMC minus sign problem. Indeed, it remains an open and challenging problem as to whether such complete or even partial sign rules can be found for other highly correlated lattice systems which also suffer from the minus sign problem. Of particular interest, for example, would be to attempt to extend our work to both electron-lattice models and frustrated spin-lattice models.

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