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MARSHALL-PEIERLS SIGN RULES, THE QUANTUM MONTE CARLO METHOD, AND FRUSTRATION

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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-neighbour pair once and once only, 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 neighbours 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 Ising representation. The coefficients $\{c_I\}$ were proven to have the property that, $c_I = (-1)^{\phi(I)} a_I$, 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, $\phi = n_A$, which counts all of the spin-half 'up' states on the A -sublattice. Lieb and Mattis² proved that the ground state of the HAF was a singlet, following the work of Marshall¹ and Lieb *et al.*³

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

$$H' = e^{i\pi\phi} H e^{-i\pi\phi}. \quad (3)$$

It is seen that H' of Eq. (3) contains only non-positive 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 non-degenerate. 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. Amongst these theorems was one which stated that the ground-state expectation value of $\mathbf{s}_i \cdot \mathbf{s}_j$ for these models is positive or negative depending on whether i and j are on the same or different sublattices, respectively.

We now attempt to extend these earlier results to other models. The first model

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

$$H_{XYZ} = \sum_{[i,j]} \left\{ J_{i,j}^x s_i^x s_j^x + J_{i,j}^y s_i^y s_j^y + J_{i,j}^z s_i^z s_j^z \right\},$$

$$= \sum_{[i,j]} \left\{ a_{i,j} s_i^z s_j^z + b_{i,j} (s_i^+ s_j^- + s_i^- s_j^+) + c_{i,j} (s_i^+ s_j^+ + s_i^- s_j^-) \right\}, \quad (4)$$

where $a_{i,j} = J_{i,j}^x$, $b_{i,j} = (J_{i,j}^x + J_{i,j}^y)/4$ and $c = (J_{i,j}^x - J_{i,j}^y)/4$. The index i in Eq. (4) 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

$$H_{SIA} = \sum_{[i,j]} J_{i,j} \left\{ s_i^z s_j^z + \frac{1}{2} (s_i^+ s_j^- + s_i^- s_j^+) \right\}$$

$$+ \frac{D}{4} \sum_i \left\{ (s_i^+)^2 + (s_i^-)^2 + 2(s(s+1) - (s_i^z)^2) \right\}. \quad (5)$$

Again, the index i in Eq. (5) 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

$$H_{TIM} = \sum_{[k_1, k_2]} \Omega_{k_1, k_2} s_{k_1}^z s_{k_2}^z + \frac{\lambda}{2} \sum_i (s_i^+ + s_i^-). \quad (6)$$

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, note that adding extra diagonal terms in Eqs. (4-6) (such as an external magnetic field or crystal field anisotropy in the z -direction), or letting i and j in Eqs. (4) and (5) run over the same sublattice but, in this case, explicitly restricting $b_{i,j} \leq 0$ in Eq. (4) and $J_{i,j} \leq 0$ in Eq. (5), do not change the following sign rules.

We now define the following operators,

$$m_A = \sum_{l_A} s_{l_A}^z; \quad m = \sum_l s_l^z, \quad (7)$$

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 $|I\rangle = \bigotimes_{l=1}^N |s_l, m_l\rangle$, where $s_l^z |s_l, m_l\rangle = m_l |s_l, m_l\rangle$, 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 signs of the $\{c_I\}$ coefficients for the expansion of the ground-state wave functions, Eq. (2), of the anisotropic Hamiltonians of Eqs. (4-6). The sign rules are

thus defined by,

$$\left. \begin{array}{ll} \phi = 1 & ; \text{ rule (A)} \\ \phi = m_A & ; \text{ rule (B)} \\ \phi = m/2 & ; \text{ rule (C)} \\ \phi = m_A + m/2 & ; \text{ rule (D)} \\ \phi = m & ; \text{ rule (E)} \end{array} \right\} \quad (8)$$

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

$$\left. \begin{array}{lll} \text{Rule} & \text{XYZ model} & \text{SIA model} \\ \text{(A)} & b_{i,j} \leq 0, c_{i,j} \leq 0 & D \leq 0, J_{i,j} \leq 0 \\ \text{(B)} & b_{i,j} > 0, c_{i,j} \geq 0 & D \leq 0, J_{i,j} > 0 \\ \text{(C)} & b_{i,j} \leq 0, c_{i,j} > 0 & D > 0, J_{i,j} \leq 0 \\ \text{(D)} & b_{i,j} > 0, c_{i,j} < 0 & D > 0, J_{i,j} > 0 \end{array} \right\} \quad (9)$$

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. (4) or (5).) 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. (6). The effect of these sign rules and the transformation of Eq. (3) is now that,

$$\langle I_1 | (H' - w) | I_2 \rangle \leq 0 \quad \forall \quad I_1, I_2; \quad (10)$$

where w is a positive number large enough to force the diagonal elements to be always negative. Note that the following relationship *also* holds:

$$\langle I_1 | \exp[\alpha(H' - w)] | I_2 \rangle \geq 0 \quad \forall \quad I_1, I_2; \quad \text{if } \alpha \leq 0. \quad (11)$$

The ground-state eigenvector of H may be written as, $|\Psi\rangle = \sum_I \exp[-i\pi\phi(I)] a_I |I\rangle$, where $a_I \geq 0 \quad \forall \quad I$. 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.

We now turn our attention to quantum Monte Carlo (QMC) calculations. 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, $p(I, I') \equiv \langle I | G | I' \rangle \Phi(I') / \Phi(I) > 0$, on the probability $p(I, I')$ for a walker to make a transition from an initial configuration $|I\rangle$ to another configuration $|I'\rangle$ along a random walk, where $\Phi(I)$ is the wave function of the initial trial state. If we choose $G \equiv \exp[-\tau(H' - w)]$, with $\tau \geq 0$ and $\Phi(I) \geq 0 \quad \forall \quad I$, we may see from Eq. (11) that this is indeed satisfied.

Finally, we note that sign rules are difficult to prove when off-diagonal terms in the Hamiltonian compete against each other (i.e., frustration). However, one may

Figure 1. Ising expansion coefficients corresponding to two-body excitations plotted against lattice distance, R , for the triangular lattice HAF using the CCM technique.

use approximate methods, such as the coupled cluster method⁸ (CCM), in order to probe the nodal surface in the Ising basis. The CCM ground-state ket wave function is given by,

$$|\Psi\rangle = e^S |\Phi\rangle, \quad (12)$$

where $|\Phi\rangle$ is the model state. Eqs. (2) and (12) are used in order to obtain approximate values for $\{c_I\}$. Fig. 1 plots these for two-body excitations with respect to $|\Phi\rangle$ as a function of the lattice distance, R , for the spin-half Heisenberg antiferromagnet (HAF) on the triangular lattice, for which exact results are not known. The LSUB m approximation, which includes all m -body (or lower-order) correlations in S in a locale also defined by m , and the SUB2 approximation, which includes all two-body correlations in S but with no further restriction on the lattice distance, are utilised in these calculations.⁸ Hence, the CCM is simulating from an *ab initio* point-of-view the nodal surface of this frustrated spin model.

References

1. W. Marshall, *Proc. Roy. Soc. A* **232**, 48 (1955).
2. E. H. Lieb and D. C. Mattis, *J. Math. Phys.* **3**, 749 (1962).
3. E. H. Lieb, T. D. Schultz, and D. C. Mattis, *Ann. Phys. (N. Y.)* **16**, 407 (1961).
4. O. Perron, *Math. Ann.* **64**, 248 (1907); G. Frobenius, *Sitzungsber. Preuss. Akad. Wiss. (Berlin) Math.-Nat. Kl.* 471 (1908); R. A. Horn and C. R. Johnson, *Matrix Analysis* (Cambridge University Press, Cambridge, 1985).
5. R. G. Munro, *Phys. Rev. B* **13**, 4875 (1976).
6. J. B. Parkinson, *J. Phys. C: Solid State Phys.* **10**, 1735 (1977).
7. D. J. Klein, *J. Chem. Phys.* **77**, 3098 (1982).
8. R. F. Bishop, D. J. J. Farnell, and Chen Zeng, *Phys. Rev. B* **59**, 1000 (1999).