TITLE: A QUANTUM MONTE CARLO STUDY OF A SPIN $-\frac{1}{2}$ CHAIN

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A Quantum Monte Carlo Study of a Spin $-\frac{1}{2}$ Chain

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Abstract

An efficient finite temperature Quantum Monte Carlo simulation is described for nearest neighbor spin-$\frac{1}{2}$ models in the presence of external magnetic fields. The method is used to study the specific heat and susceptibility of ferromagnetic easy plane cases with an in-plane magnetic field, and applied to the one-dimensional magnet $(C_6H_{11}NH_3)CuBr_3$.

A number of one dimensional (1-D) model spin systems have been studied recently using finite temperature quantum Monte Carlo (QMC) methods.[1,2,3] Cullen and Landau[2] have studied the isotropic spin-$\frac{1}{2}$ Heisenberg chain and the analytically solvable XY model using the "checkerboard decomposition". Both of these systems have been mapped to 6-vertex models. We would like to extend and apply their methods to spin-$\frac{1}{2}$ systems in which the exchange is anisotropic, in particular with easy plane anisotropy, and where there is an applied magnetic field in the easy plane. The addition of these two symmetry breaking terms is shown below to lead to either an 8 or 16 vertex model, depending on the set of eigenstates chosen, and these can be more efficient to work with than the 6-vertex models.

There has been some experimental evidence that an example of this type of system, the spin-$\frac{1}{2}$ ferromagnet "CHAB" (($C_6H_{11}NH_3$)$CuBr_3$) shows thermodynamic properties indicative of sine Gordon soliton-like excitations.[4] The magnetic field and temperature dependences of the measured specific heat has been fitted to classical sine-Gordon theory with a renormalized rest mass, but a priori this seems of doubtful validity in such a low spin system where quantum effects should have great importance. The purpose here is to obtain the low temperature thermodynamics for this system without making any classical approximations, in order to investigate the physical importance of quantum effects and directly assess the accuracy of the presumed Hamiltonian. Another similar real material exists, $CsNiF_3$, which is a spin-1 easy-plane ferromagnet in which the exchange is believed to be isotropic but there is a single ion easy plane anisotropy.[5,6] A similar QMC study of that system will be reported elsewhere.

The general N spin Hamiltonian we consider is

$$\hat{H} = - \sum_{i=1}^{N} (J_x \hat{S}_i^x \hat{S}_{i+1}^x + J_y \hat{S}_i^y \hat{S}_{i+1}^y + J_z \hat{S}_i^z \hat{S}_{i+1}^z) \tag{1}$$

$$- \sum_{i=1}^{N} [\frac{1}{2} h_x (\hat{S}_i^x + \hat{S}_{i+1}^x) + \frac{1}{2} h_z (\hat{S}_i^z + \hat{S}_{i+1}^z)] = \sum_{i=1}^{N} \hat{H}_{i,i+1}$$

Here $\hat{S}_i^x$, $\hat{S}_i^y$, $\hat{S}_i^z$ are spin-$\frac{1}{2}$ operators, J_x, J_y, J_z, are arbitrary exchange constants, and h_x, h_z are applied fields. We use a transformation first proposed by Suzuki[1] which uses the Trotter formula to map this 1-D quantum Hamiltonian onto an approximately equivalent 2-D classical Hamiltonain. For further details see references (1,2,3,7). First the two-site Hamiltonian $\hat{H}_{i,i+1}$ is written as the sum of two noncommuting parts (to simplify evaluation of matrix elements later):

$$\hat{H}_{i,i+1} = \hat{H}^0_{i,i+1} + \hat{V}_{i,i+1}$$

$$\hat{H}^0_{i,i+1} = - J_z \hat{S}_i^z \hat{S}_{i+1}^z - \frac{1}{2} h_z (\hat{S}_i^z + \hat{S}_{i+1}^z) \tag{2}$$

$$\hat{V}_{i,i+1} = - J_x \hat{S}_i^x \hat{S}_{i+1}^x - J_y \hat{S}_i^y \hat{S}_{i+1}^y - \frac{1}{2} h_x (\hat{S}_i^x + \hat{S}_{i+1}^x)$$

The partition function $Z = $ trace $\{e^{-\beta \hat{H}}\}$, where $\beta = 1/T$ and T is the temperature, is approximated using the mth order Trotter formula within the trace. The resulting mth order approximation for Z, denoted $Z^{(m)}$, is

$$Z^{(m)} = \left(\sum_{\text{all } S_{i,r} = \pm\frac{1}{2}} \right) \langle \prod_{i=1}^{N} \prod_{r=1}^{2m} e^{-\beta E^{(m)}(i,r)} \rangle , \tag{3}$$

where the bracket notation < > means only those terms where i,r are both odd or both even are included. (This is the origin of the term "checkerboard decomposition"). The vertex energy $E^{(m)}(i,r)$ for the vertex (block of four spins) at site (i,r) in the 2-D lattice is given by

$$e^{-\beta E^{(m)}(i,r)} = \langle S_{i,r} S_{i+1,r} \left| e^{-\frac{\beta \hat{H}^0_{i,i+1}}{2m}} \; e^{-\frac{\beta \hat{V}_{i,i+1}}{m}} \; e^{-\frac{\beta \hat{H}^0_{i,i+1}}{2m}} \right| S_{i,r+1} S_{i+1,r+1} \rangle \; ,$$

(4)

Here the $S_{i,r}$ are eigenvalues of an appropriately chosen operator. We have approximated $e^{-\frac{\beta \hat{H}_{i,i+1}}{m}}$ in a symmetric way, in order to preserve the invariance of the matrix elements with respect to the interchange of r and $r + 1$. In the limit $m \to \infty$, $Z^{(m)}$ approaches the exact partition function of the original 1-D quantum problem.

At each of the N x 2m sites in this lattice there is an Ising spin variable $S_{i,r} = \pm \frac{1}{2}$, the eigenvalue of $\hat{S}^z_i$ in the $\underline{r}$th set of states used in the Trotter approximation. (We quantize using eigenstates of $\hat{S}^z_i$). This effective 2-D lattice has periodic boundary conditions in the "Trotter direction" (the "r", or path integral, direction) as a result of the trace operation, while we impose periodic boundary conditions in the spatial direction. These spins, taken in blocks of four, determine the energies of the $\frac{1}{2}Nm$ vertices on the lattice, and therefore the total energy in the 2-D system.

Since we are using eigenstates of $\hat{S}^z_i$ operators, matrix elements of $e^{-\frac{\beta \hat{H}^0_{i,i+1}}{m}}$ are trivial. For those of $e^{-\frac{\beta \hat{V}_{i,i+1}}{m}}$, we make use of the operator identity[8]:

$$2 \exp -\frac{\beta \hat{V}_{i,i+1}}{m} = \left[e^{K_x}(\cosh K_b - \gamma \sinh K_b) + e^{-K_-} \right] \left(\frac{1+\hat{\sigma}_i^z \hat{\sigma}_{i+1}^z}{2} \right)$$

$$+ \left[e^{K_x}(\cosh K_b + \gamma \sinh K_b) + e^{-K_+} \right] \left(\frac{1-\hat{\sigma}_i^z \hat{\sigma}_{i+1}^z}{2} \right)$$

$$+ \left[e^{K_x}(\cosh K_b + \gamma \sinh K_b) - e^{-K_+} \right] (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)$$

$$+ \left[e^{K_x}(\cosh K_b - \gamma \sinh K_b) - e^{-K_-} \right] (S_i^+ S_{i+1}^+ + S_i^- S_{i+1}^-)$$

$$+ \left[2\alpha\gamma e^{K_x} \sinh K_b \right] (S_i^+ + S_i^- + S_{i+1}^+ + S_{i+1}^-) \quad , \quad (5)$$

where $\hat{\sigma}_i^z = 2\hat{S}_i^z$, S_i^+ and S_i^- are raising and lowering operators, and

$$K_{x,y,z} \equiv \frac{\beta J_{x,y,z}}{4m} \quad ; \quad K_{\pm} = K_x \pm K_y \quad ; \quad \alpha = \frac{h_x}{J_y} = \frac{b_x}{K_x} \quad ;$$

$$b_{x,z} = \frac{\beta h_{x,z}}{4m} \quad ; \quad \gamma = \frac{1}{\sqrt{1+4\alpha^2}} \quad ; \quad K_b = \frac{K_y}{\gamma} \quad (6)$$

It will be seen that of the 16 possible vertices, all are nonzero if $h_x \neq 0$ (16 vertex model), while 8 are nonzero if $h_x = 0$ and $J_x \neq J_y$ (8 vertex model). Only 6 are nonzero if $h_x = 0$ and $J_x = J_y$ (the isotropic 6 vertex model in Ref. 2). Thus the presence of symmetries tends to reduce the number of allowed vertices -- vertex weights which are zero correspond to infinite energy and therefore prohibited states. If any weight is negative or complex, the energy is complex. Such vertices are not prohibited if they always occur in pairs, such that their net contribution to $Z^{(m)}$ is real and positive. This is always the case for the 8 vertex model.

In principle the simplest model with which one can work, is the 16 vertex model, since individual spin flips can then be the basic QMC "move". An 8 vertex model is also convenient; there the basic moves are row, column, and square flips. (These types of moves always generate allowed states). For a 6 vertex model, we do not know a set of simple moves which keeps one within the 6 allowed vertices, so that using a combination of row, column, and square flips can generate disallowed states and waste computing time. Ironically the presence of too much symmetry in the original problem makes the case of isotropic exchange with only a field parallel to the quantization axis the most difficult in the present formalism.

The specific heat of CHAB has been measured[4] in the temperature range from 1.7 to 7K, with a transverse field up to 7kG (approx. 1K). For the parameter values believed[4] to be associated with CHAB: $J_x = J_y = 110K$, $J_z = 104.5K$, and for fields $h_z = 0$, $0 < h_x \leq 10kG$, one finds that although this is a 16 vertex model, the percentage of single spin flip moves accepted using the standard Metropolis algorithm is impractically small (less than 1% for $1K \leq T \leq 10K$). This is because this model is approximately a 6 vertex model, with the magnetic field just a mild perturbation. The 16 vertex model works well only if the field, exchange constants, and temperature are all the same order of magnitude.[9]

An alternative way to study the thermodynamics for CHAB is to choose $J_x = J_z = 110K$, and $J_y = 104.5K$, $h_x = 0$, $0 \leq h_z \leq 10kG$. (That is, rotate the coordinate system so that the quantization axis lies in the easy plane). This is now an 8 vertex model, and remains an 8 vertex model even when the field goes to zero. Provided the anisotropy is

strong enough, this will be a good 8 vertex model to work with rather than just a small perturbation on a 6 vertex model. This is the model for which we have performed a QMC calculation. In this case it is interesting to remark on the effective Hamiltonian for the 2-D lattice. (The general case is given in Ref. 8). The vertex energy $E^{(m)}(i,r)$ can be written (for the 8 allowed vertices)

$$E^{(m)}(i,r) = J_h(S_{i,r}S_{i+1,r} + S_{i,r+1}S_{i+1,r+1}) + J_v(S_{i,r}S_{i,r+1} + S_{i+1,r}S_{i+1,r+1})$$

$$+ J_d(S_{i,r}S_{i+1,r+1} + S_{i+1,r}S_{i,r+1}) - \frac{b_z}{\beta}(S_{i,r} + S_{i+1,r} + S_{i,r+1} + S_{i+1,r+1})$$

$$(8)$$

Thus the effective 2-D Hamiltonian has different near neighbor couplings in the real space (J_h) and Trotter (J_v) directions, and in addition a second nearest neighbor diagonal interaction (J_d). The exchange constants are

$$J_h = (2\beta)^{-1} \ln[e^{-4K_z} \sinh2K_+/\sinh2K_-]$$

$$J_v = (2\beta)^{-1} \ln[\tanh K_+ \tanh K_-]$$

$$(9)$$

$$J_d = (2\beta)^{-1} \ln[\tanh K_-/\tanh K_+]$$

For CHAB at very low temperature, all three exchange constants are negative. However, as the temperature is increased J_h becomes positive and we have a system with competing ferromagnetic and antiferromagnetic interactions.

The Monte Carlo Algorithm: Within the 8 vertex model, one must always flip the spins at a vertex in pairs, and this necessitates flipping a series of spins in the lattice which lie on a closed path. We have chosen to use a combination of straight column flips plus square flips, especially since the staggered column flips of Ref. 2 can always be decomposed into a series of square flips plus one straight column flip. Row flips have very low acceptance rates and so are not used.

In a single MC step, we attempt N column flips and $\frac{1}{2}Nm$ square flips, chosen at random positions. Typical simulations used from $10^5 - 3 \times 10^5$ steps, with the first 20% disregarded, and the rest split into groups for error analysis. The internal energy, specific heat, magnetization, and susceptibility were computed as in Ref. 2 from expectation values of appropriate derivatives of the vertex weights. The validity of the algorithm was checked by comparison with an exact $m = 1$ transfer matrix calculation.

An initial configuration of the system was obtained by first taking a small number of MC steps at a temperature which was twice the desired value, in order to "stir" the system. The data obtained using several such initial states was then averaged to produce the results shown here. We have used $N = 32$, and $m = 2, 4, 8, 12$ and 16. For the present case, we have found that the choice of $m = 8$ is the optimum value for which the statistical errors are reasonably small ($\sim$ 5% for available computing time), and the error due to using a finite m Trotter approximation seems to be of similar magnitude.

Susceptibility measurements for CHAB are not available but accurate specific heat studies have been made.[4] Our results for ΔC, Fig. 1(c), are in fair agreement with the experimental data regarding the

temperatures at which ΔC maximizes. Comparison with the Ref. 4 results shows that the most obvious differences are a tendency for the QMC results to lie below the experimental ones for ΔC -- by approximately 20%. This could have several sources: (i) A systematic additional specific heat component measured experimentally, e.g. nonmagnetic contributions or entropy-reducing pinning effects in the absence of a field (ii) Errors in the parameter values assumed in the model Hamiltonian (1), or corrections to the Hamiltonian. Regarding the parameter values, these have been estimated primarily[4] from fits to linear properties. There is a possibility that more accurate assignments of parameters are necessary before precise comparisons with classical or quantum "soliton" theories can be made, especially for such sensitive properties as ΔC. We have investigated the effect of varying the easy plane anisotropy from 3% to 7% (5% being assumed previously). While decreasing the anisotropy decreases C, any systematic variations in ΔC are small, less than the error bars for ΔC, which are approximately ±15%. (iii) Finally, there may be systematic QMC errors leading to an underestimate of C and ΔC, especially due to finite m Trotter approximation. Work in progress on an "exact" transfer matrix calculations and on computer renormalization calculations for finite chains may help to answer this question. Also, comparisons with data[5] for ΔC in the _spin-1_ ferromagnetic $CsNiF_3$ are in progress and should throw further light on the question of how accurately simple model Hamiltonians describe the magnetic behaviors and how well parameter values are known. These are very important questions in view of the continuing controversies[6] concerning the use of classical or quantum theories in either CHAB or $CsNiF_3$.

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9. A single spin flip in a vertex causes a transition from a vertex with an odd (even) number of $+\frac{1}{2}$'s to a vertex with an even (odd) number of $+\frac{1}{2}$'s. When the field is small compared to the exchange, vertices with an odd number of $+\frac{1}{2}$'s have energies much larger than the other vertices, and single spin flip acceptance rates rapidly approach zero. This is the major source of difficulty with this 16 vertex model.

Fig. 1 QMC results for CHAB at fields h_z = 0.0(o), 3.3(Δ), 6.5(+), 10.0(x) kG. The data points in (a) were found from expectation values of the variable $\frac{\partial}{\partial \beta}(\beta E^{(m)}(i,r))$, while those in (b) were the fluctuations in this variable. The curves in (a) are weighted least squares polynomial fits to the data points, while the curves in (b) are derivatives of the fitted curves in (a). In (c) we also show the difference $\Delta C(T)$ -- the specific heat with a field minus the zero field result, obtained directly from (b). Finally (d) shows the susceptibility in the direction of the applied field (in the easy plane); the curves are polynomial fits to the reciprocal susceptibility.