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A New Approach to Quantum Spin-Systems: The Critical Properties of a Heisenberg Ferromagnet

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The critical temperature and exponents of a three-dimensional, spin-$\frac{1}{2}$, quantum Heisenberg ferromagnet are obtained using a new method. A simple cubic lattice of L^3 sites with periodic boundary conditions is considered. The Heisenberg Hamiltonian is

$$H = J \sum_{\mathbf{j},\delta} \mathbf{S}_\mathbf{j} \cdot \mathbf{S}_{\mathbf{j}+\delta}$$

where δ is a vector connecting nearest-neighbor sites. The spin operators at site $\mathbf{j}$ are $\mathbf{S}_\mathbf{j} \equiv (\hbar\mu_B/2)(\sigma^x, \sigma^y, \sigma^z)_\mathbf{j}$, where the $\sigma^{x,y,z}$ are the Pauli matrices and μ_B is the Bohr magneton.

Fourier transforming to a wave-number space allows a parametrization of the system in terms of spin-wave states, each spin-wave being an excitation at a wave-number $\mathbf{k}$. Working in occupation number space the states of the system are defined by a set $\mathbf{n}(\mathbf{k}) = [n(\mathbf{k}_1), n(\mathbf{k}_2), \ldots]$ of occupation numbers giving the number of spin-waves at each $\mathbf{k}$; $\mathbf{n}$ takes integer values over the discrete wave-number field.

Given a state $|\mathbf{n}\rangle$, the expectation value of the absolute magnetization is given by

$$\mathbf{M} = \left[\langle \mathbf{n} | \left(\sum_\mathbf{i} \mathbf{S}_\mathbf{i} \right) \cdot \left(\sum_\mathbf{j} \mathbf{S}_\mathbf{j} \right) | \mathbf{n} \rangle \right]^{1/2} = [S_{\max}^2 - Q(N+1-Q)]^{1/2}$$

where $N \equiv L^3$, $S_{\max}^2 = (N/2)[(N/2)+1]$, and $Q = \sum_{k \neq 0} n(k)$. The thermal

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expectation value of the susceptibility is computed from the fluctuation dissipation theorem as

$$\chi_\beta = \frac{N}{k_B T}[\langle \mathbf{M}^2 \rangle_\beta - \langle \mathbf{M} \rangle_\beta^2] \tag{1}$$

Where $\langle x \rangle_\beta$ is the thermal expectation value of x at $\beta = 1/(k_B T)$.

The simulation proceeds by generating states in the occupation number space (Fock space) which are assigned free spin-wave energies

$$E(\mathbf{n}) = n(\mathbf{k}_1)\, E(\mathbf{k}_1) + n(\mathbf{k}_2)\, E(\mathbf{k}_2) + \cdots \tag{2}$$

where $E(\mathbf{k}) = J[3 - \cos(k^x 2\pi/L) - \cos(k^y 2\pi/L) - \cos(k^z 2\pi/L)]$. The initial state is taken to be the ground state where $n(\mathbf{k}) = 0$ for all $\mathbf{k}$ and the updating is performed by sweeping through k space. At each point k_0 a new occupation number $n'(k_0)$ is constructed as the old occupation number plus or minus a randomly chosen, nonzero interger Δ. The probability of Δ taking a particular value is uniformly distributed over the range of integers from $-\Delta_{\max}$ to $+\Delta_{\max}$, excluding zero, and equals zero outside this range and at $\Delta = 0$. The step width $\Delta_{\max}$ is chosen to optimize the convergence of the simulation

$$n'(k_0) = n(k_0) + \Delta$$

Two important restrictions are imposed on the space of occupation numbers. First, no occupation number can be negative, as this would lead to unphysical states with energies less than the ground state. Second, the total number of excitations n_{tot} must be less than or equal to half the number of sites in the system

$$\begin{aligned} n(\mathbf{k}) &\geqslant 0 \qquad \text{for all } \mathbf{k} \\ n_{\text{tot}} &\equiv \sum_{\mathbf{k}} n(\mathbf{k}) \leqslant L^3/2 \end{aligned} \tag{3}$$

This second condition derives from the fact that no more than L^3 spin-waves can be excited in a system of L^3 sites. In addition, in a zero external field, the set of spin-waves excited from a ground state with all spins pointing down and spin-waves excited from a ground state with all states pointing up are degenerate in energy and absolute value of magnetization. From (1) these two sets also give the same contribution of the susceptibility. As a result, it is only necessary to consider the space consisting of half the maximum number of excitations. Hence the upper limit $L^3/2$. Whenever a state is generated in the underlying Markov chain that violates the conditions in (3) it is treated as having an infinite energy.

The results of the Monte Carlo simulation for sustems of 3^3, 5^3, 7^3, 9^3, and 15^3 sites were analyzed according to finite-size scaling theory. This

Table I. Critical Temperature and Exponents According to Mean-Field Theory, High-Temperature Expansions, and the Present Spin-Wave Theory

	Mean field	High-temperature series	Spin-wave
T_C	3	$1.68 \pm .01$	$1.53 \pm .02$
β	.50	$.385 \pm .025$	$.63 \pm .02$
γ	1.00	$1.43 \pm .01$	$4.1 \pm .2$

theory says that for sufficiently large systems near the critical region the following relations hold

$$\begin{aligned} \mathbf{M}(N, t) &\propto N^a (tN^b)^\beta \\ \chi(N, t) &\propto N^c (tN^d)^{-\gamma} \qquad \text{where} \quad t \equiv T_C - T \end{aligned} \tag{4}$$

T_C is the temperature at which the susceptibility of the infinite system is singular, as extrapolated from the peaks in the susceptibilities of the finite-size results; a, b, c, and d are chosen so as to best satisfy the scaling relations. In the t region where scaling relations hold, $\log[N^{-a}\mathbf{M}(N, t)]$ and $\log[N^{-c}\chi(N, t)]$ are linear functions of $\log(tN^b)$ and $\log(tN^d)$. The critical exponents β and $-\gamma$ are read off as the slopes of $\log[N^{-a}\mathbf{M}(N, t)]$ and $\log[N^{-c}\chi(N, t)]$ plotted against $\log(tN^b)$ and $\log(tN^d)$. γ is obtained from χ below T_C. In Table I these results, with those obtained from mean-field theory and high-temperature expansions, are shown.

These results are surprisingly good considering the simplicity of the model.

Several features of this approach are of note. First, critical behavior is exhibited by a noninteracting particle model. Second, we do not observe any critical slowing down in the convergence of the Monte Carlo simulations. This can be ascribed to working in k space where every configuration includes the effects of the position-space boundaries. Third, we have predicted the behavior of a three-dimensional quantum system by performing Monte Carlo simulations in a three-dimensional classical configuration space. This is to be contrasted with previous quantum Monte Carlo work which transcribes d-dimensional quantum system into $d+1$ dimensional classical systems and, therefore, requires computation times that are greater by a factor of the system size.