Multichain Mean-Field Theory of Quasi-One-Dimensional Quantum Spin Systems

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A multichain mean-field theory is developed and applied to a two-dimensional system of weakly coupled $S = 1/2$ Heisenberg chains. The environment of a chain C_0 is modeled by a number of neighboring chains C_δ, $\delta = \pm 1, \ldots, \pm n$, with the edge chains $C_{\pm n}$ coupled to a staggered field. Using a quantum Monte Carlo method, the effective $(2n + 1)$-chain Hamiltonian is solved self-consistently for n up to 4. The results are compared with simulation results for the original Hamiltonian on large rectangular lattices. Both methods show that the staggered magnetization M for small interchain couplings α behaves as $M \sim \sqrt{\alpha}$ enhanced by a multiplicative logarithmic correction.

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Quasi-one-dimensional (quasi-1D) quantum spin systems have become an important field of study in solid state physics. Many unusual, theoretically predicted properties of 1D systems have been observed in real materials. For example, the gapless two-spinon spectrum [1] of the $S = 1/2$ Heisenberg chain has been observed in neutron scattering experiments on $KCuF_3$ [2], and the Haldane gap predicted for integer S [3] has been detected, e.g., in the $S = 1$ compound $CsNiCl_3$ [4]. Quantum critical scaling [5] has been observed in the NMR relaxation rates of the $S = 1/2$ system Sr_2CuO_3 [6], possibly even including anticipated [5,7] logarithmic corrections [8]. In spite of the success of strictly 1D models for these and many other quasi-1D magnetic materials, interchain couplings can be important as well. A single isotropic chain cannot order, not even at $T = 0$, whereas a transition to a Néel ordered state is often observed at low temperature; $KCuF_3$ and Sr_2CuO_3 both order at $T_N \approx 5$ K. Interchain couplings also change qualitatively the nature of the low-lying excitations and lead to interesting dimensional crossover phenomena.

One way to take into account interchain couplings $J_\perp$ in a quasi-1D system with long-range order is to model the environment of a single chain C_0 by a staggered magnetic field [9–12]. The effective 1D system can be solved numerically on small lattices [10,12], or using analytical techniques [11]. In this Letter, the mean-field approach is extended to include also a number of neighboring chains C_δ to which C_0 is coupled. In two dimensions $\delta = \pm 1, \ldots, \pm n$. A staggered field is coupled to the edge chains $C_{\pm n}$, to model their long-range ordered environment. Fluctuations neglected in the environment of C_δ are approximated by a modification of their intrachain interactions, in such a way that self-consistency is achieved in the induced staggered magnetizations on C_0 and C_δ. The effective $(2n + 1)$-chain Hamiltonian can be solved using numerical methods, which typically perform much better for a few coupled chains than for 2D or 3D lattices.

Here these ideas will be applied to a system of antiferromagnetic Heisenberg chains, with the Hamiltonian

$$H = J \sum_{i,j} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} + J_\perp \sum_{i,j} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1}, \quad (1)$$

where $\mathbf{S}_{i,j}$ denotes a spin-1/2 operator at site i of chain j. The focus will be on the dependence of the $T = 0$ staggered magnetization $M = \langle S^z_{i,j} \rangle (-1)^{i+j}$ on the coupling constant ratio $\alpha = J_\perp / J$. The question of whether or not long-range order $(M > 0)$ develops for arbitrarily small $\alpha > 0$ has been the subject of numerous studies. Conventional spin-wave theory predicts a finite critical value α_c below which $M = 0$ [10,13], but RPA [14] gives $\alpha_c = 0$. Some self-consistent calculations predict $\alpha_c = 0$ [15], whereas others have given α_c as high as 0.2 [16]. Renormalization group analyses of the interchain interactions are associated with subtleties [17,18], and completely conclusive results have not been presented; however, $\alpha_c = 0$ appears most plausible [18,19]. An analytical treatment of the single-chain mean-field theory gave the behavior $M \sim \sqrt{\alpha}$ for small α [11,18]. Numerically, M has been calculated using exact diagonalization [13,16] and series expansion techniques [17], the former indicating $\alpha_c \approx 0.1–0.2$, and the latter giving an upper bound $\alpha_c \lesssim 0.02$. Numerical calculations have in general been hampered by convergence problems and difficult extrapolations for small α. Here multichain mean-field calculations will be complemented by large-scale quantum Monte Carlo simulations of the original 2D Hamiltonian (1). It will be shown that quadratic $(L \times L)$ lattices are not suitable for extrapolations to the thermodynamic limit when $\alpha \ll 1$, due to unusual, nonmonotonic finite-size effects. Using rectangular lattices with aspect ratios L_x/L_y as large as 16, it was, however, possible to study systems with α as low as 0.02. Both the mean-field calculations and the 2D simulations indicate that M vanishes as $\alpha \to 0$ *slower* than $\sqrt{\alpha}$, due to a logarithmic correction to this form.

In the conventional single-chain mean-field treatment of the Hamiltonian (1) [9–11], the coupling of a chain j to its nearest neighbors $j \pm 1$ is approximated by $J_\perp \sum_i S^z_{i,j}[\langle S^z_{i,j-1}\rangle + \langle S^z_{i,j+1}\rangle]$. In a Néel state $\langle S^z_{i,j}\rangle = (-1)^{i+j}M$, and one obtains an effective 1D Hamiltonian,

$$H_1 = J \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} - h \sum_i (-1)^i S^z_i \,, \qquad (2)$$

with the self-consistency condition $h = 2J_\perp M$ which directly relates $M(h)$ to $M(J_\perp)$ of the 2D system.

The idea of the multichain mean-field theory is to model the environment of a chain C_0 by its first few neighbor chains C_δ, $\delta = \pm 1, \ldots, \pm n$, with only the edge chains $C_{\pm n}$ coupled to a staggered field. This induces a staggered magnetization in all chains. The dynamic environment for C_0 provided by the C_δ chains should be considerably more realistic than just the static staggered field of the single-chain theory. If C_0 and C_δ are identical chains, it is not possible to obtain a self-consistent description, however. The staggered magnetization will be largest at the edges and decrease towards the center, due to the neglected quantum fluctuations at the edges. These fluctuations can be approximated by a modification of the intrachain interactions of C_δ. There are clearly many possible ways of doing this, and the optimum way that would best mimic the presence of an infinite half-plane of other chains is not obvious. One requirement is that the additional interactions have to be invariant under spin rotations in the xy plane [since the field breaks the $O(3)$ symmetry, an $O(2)$ symmetric effective interaction in C_δ is permissible]. Here the simplest interaction satisfying this requirement will be considered; namely, the xy part of the coupling is given a strength $J^{xy}_\delta = J(1 + \lambda_{|\delta|})$ different from $J^z_\delta = J$. Increasing $\lambda_{|\delta|} > 0$ increases the quantum fluctuations. The $(2n + 1)$-chain effective Hamiltonian is then

$$\begin{aligned} H_n = {} & J \sum_{i=1}^{L} \sum_{j=-n}^{n} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} + J_\perp \sum_{i=1}^{L} \sum_{j=-n}^{n-1} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1} \\ & + \sum_{i=1}^{L} \sum_{\delta=\pm 1}^{\pm n} \lambda_{|\delta|}(S^x_{i,\delta}S^x_{i+1,\delta} + S^y_{i,\delta}S^y_{i+1,\delta}) \\ & + h \sum_{i=1}^{L} (-1)^i (S^z_{i,-n} + S^z_{i,n}) \,. \end{aligned} \qquad (3)$$

There are $n + 1$ self-consistency conditions,

$$M \equiv M_0 = M_1 =, \ldots, = M_n = h/J_\perp \,. \qquad (4)$$

Since the environment of a chain C_k becomes more similar to that of the real 2D system the closer it is to the center ($k = 0$) of the effective $2n + 1$ chain system, the self-consistent parameters can be expected to satisfy $0 < \lambda_1 < \cdots < \lambda_n$. For a given α, the magnetization (as well as other properties) should converge to its correct value as $n, L \to \infty$. Therefore, the details of the intrachain interactions used to achieve self-consistency can be seen to be unimportant; they will affect only the rate of convergence with increasing n.

Here quantum Monte Carlo results for the cases $n = 1, 2, 3$, and 4 will be presented. In addition, results will be shown for the conventional single-chain effective Hamiltonian (2), which corresponds to $n = 0$. This 1D Hamiltonian has been studied by Schulz via a mapping to a solvable fermion model in the continuum limit [11], with the result $M = 0.719\sqrt{\alpha}$ for the 2D system. The mapping has not been demonstrated rigorously, however, and the above form of M can furthermore be valid only for small α. Numerical calculations have previously been carried out for $L \leq 10$ [10], which is not sufficient for addressing the behavior for $\alpha \ll 1$ in the thermodynamic limit.

Before presenting the mean-field results, quantum Monte Carlo calculations for the full 2D Hamiltonian (1) will be discussed. For the spatially isotropic system ($\alpha = 1$), very accurate results for M have previously [20] been obtained using ground state results for the staggered structure factor,

$$S(\pi, \pi) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \langle S^z_i S^z_j \rangle (-1)^{(x_i - x_j + y_i - y_j)}. \qquad (5)$$

Accounting for rotational averaging, the sublattice magnetization is given by

$$M^2 = 3S(\pi, \pi)/N \qquad (N \to \infty) \,. \qquad (6)$$

Here this quantity will be extrapolated to infinite size for $\alpha < 1$. Using the stochastic series expansion method with an efficient cluster update [21], systems with several thousand spins were studied. Inverse temperatures $\beta = J/T$ as high as 2048 were used in order to obtain results free of temperature effects.

For $\alpha = 1$, the leading finite-size correction to M^2 as defined in Eq. (6) is positive and $\sim 1/\sqrt{N}$ [20]. This can be expected also for $0 < \alpha < 1$ if the system is ordered. Figure 1 shows results for $\alpha = 0.05$ on $L \times L$ lattices with L up to 40. The results extrapolate to $M > 0$, but subleading corrections to the linear behavior are clearly large. Previously, results for smaller L were used as evidence that M vanishes below a critical value $\alpha_c \sim 0.1$–0.2 [13,16]. Results for rectangular lattices with different aspect ratios $R = L_x/L_y$ reveal a considerable dependence on R, as also shown in Fig. 1. For $R = 8$, the expected linear behavior can be seen clearly, and for $R = 4$ there is a crossover to this behavior for large systems. For $R = 2$ there is a clear minimum, and the $R = 1$ results also suggest one. In the two latter cases the finite-size behavior is hence nonmonotonic, and there has to be a maximum for even larger systems before the asymptotic, linear (with positive slope) approach to the infinite-size value, which for $\alpha = 0.05$ is $S(\pi, \pi)/N \approx 0.0056$ (from an extrapolation of the $R = 8$ data).

The nonmonotonicity can be understood as resulting from a crossover from 1D to 2D behavior. A chain of length L_x has an excitation gap $\Delta(L_x) \sim 1/L_x$. If this gap is larger than the effective energy scale of the coupling of the chains, i.e., the spin-stiffness ρ^y_s, then the system essentially behaves as a system of 1D chains, with

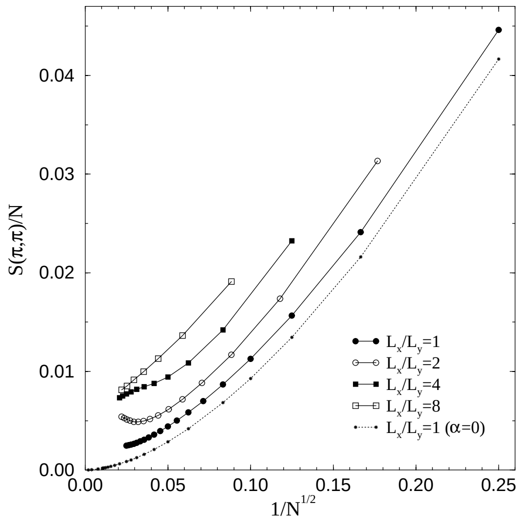

FIG. 1. Quantum Monte Carlo results for the staggered structure factor on rectangular lattices with different aspect ratios and $\alpha = 0.05$. The behavior for an $L \times L$ lattice with $\alpha = 0$ (independent 1D chains) is also shown. Statistical errors are much smaller than the symbols.

exponentially damped correlations between the chains. A crossover to 2D behavior can be expected when $\Delta(L_x) \sim \rho_s^y$, which occurs for smaller system sizes $N = L_x L_y$ when the aspect ratio R is large, in agreement with the results in Fig. 1. When $\alpha \ll 1$ (and therefore $\rho_s^y \ll 1$), quadratic lattices therefore have to be very large for extrapolations to infinite size to be meaningful. Instead, rectangular lattices with R increasing with decreasing α should be used. Using aspect ratios as large as $R = 16$, the sublattice magnetization was calculated for α as small as 0.02. Below, the results will be compared with the single- and multichain mean-field theories.

In the single-chain theory the magnetization curve $M(J_\perp)$ is directly obtained from a calculation of $M(h)$ for the Hamiltonian (2). The effective model (3) depends explicitly on $J_\perp$, however, and for each $J_\perp$ a search for the self-consistent values $h, \lambda_1, \ldots, \lambda_n$ is required. With the Monte Carlo method used [21], the derivatives $\partial M_j/\partial h$ and $\partial M_j/\partial \lambda_k$ can also be calculated. Using these, an iterative scheme, where

$$h(m+1) = h(m) + \Delta_h(m),$$
$$\lambda_k(m+1) = \lambda_k(m) + \Delta_{\lambda_k}(m), \tag{7}$$

can be employed, starting from estimated values $h(0)$ and $\lambda_k(0)$. The self-consistency conditions (4) give the corrections $\Delta_h(m)$ and $\Delta_{\lambda_k}(m)$ as the solution of $n+1$ coupled equations, e.g., for $n = 1$,

$$\Delta_h(\partial M_0/\partial h - \partial M_1/\partial h) + \Delta_{\lambda_1}(\partial M_0/\partial \lambda_1 - \partial M_1/\partial \lambda_1) = M_1 - M_0,$$
$$\Delta_h(\partial M_0/\partial h + \partial M_1/\partial h - 2/J_\perp) + \Delta_{\lambda_1}(\partial M_0/\partial \lambda_1 + \partial M_1/\partial \lambda_1) = 2h/J_\perp - M_1 - M_0. \tag{8}$$

Self-consistency is typically achieved this way in as few as two or three iterations.

For a finite system, the self-consistent M vanishes below a critical value $\alpha_c(L)$ which decreases with increasing L. In order to study the behavior for small α very large L have to be used. The largest sizes used here were $L = 1024$ for $n = 0$, 512 for $n = 1, 2$, and 256 for $n = 3, 4$. Inverse temperatures $\beta = J/T$ as high as $2L$ were used in order to completely project out the ground state.

All results for M, including those for the original 2D Hamiltonian (1) extrapolated to infinite size, are shown divided by $\sqrt{\alpha}$ in Fig. 2. The behavior predicted by Schulz [11] using a mapping of the $n = 0$ mean-field theory to a solvable continuum model should then be a constant. The numerical results for $n = 0$ do not agree with this; instead $M_0/\sqrt{\alpha}$ appears to diverge as $\alpha \to 0$. The behavior for $\alpha \lesssim 0.4$ is closely reproduced by the form $M_0 = A_0\sqrt{\alpha}\,(1 + b\alpha)\ln^\gamma(a/\alpha)$, with $\gamma \approx 1/3$, $A_0 \approx 0.53$, $a \approx 1.3$, and $b \approx 0.1$. This result shows that the mapping of Eq. (2) to the continuum model is not exact. A reason for this could be the presence of marginally irrelevant operators, which are known to lead to logarithmic corrections to physical observables in the case $h = 0$ [22]. The results for higher n also show a similar divergent behavior, but with the available computer resources it was not possible to extend the calculations to as small α as for $n = 0$. The above logarithmic form fits quite well also all the multichain results, with *only* the overall factors A_n adjusted. This is a strong indication that the logarithmic correction survives in the 2D limit ($n \to \infty$). The curves indeed approach the results obtained using finite-size extrapolations for rectangular 2D lattices, confirming that the multichain mean-field theory converges correctly. Remarkably, the same expression that describes all the mean-field data also fits the 2D results, with the amplitude $A_{2D} \approx 0.39$.

The self-consistent values of the xy-anisotropy parameters are graphed in Fig. 3 for $n = 1, 2, 3$. For $n > 1$, the anisotropy is always largest at the edges, as expected, and rapidly decreases as the center chain is approached. The behavior for $\alpha \to 0$ suggests a very slow asymptotic decay to zero—again an indication of log corrections.

To conclude, both the multichain mean-field theory and calculations for the original Hamiltonian strongly support a critical coupling $\alpha_c = 0$, and a staggered magnetization that for small interchain couplings behaves as $M \sim \sqrt{\alpha}$ enhanced by a logarithmic correction. In the conventional single-chain mean-field theory ($n = 0$), all interchain quantum fluctuations are neglected. The 2D quantum fluctuations develop systematically in the multichain theory as n is increased. For $\alpha \ll 1$, the functional form of the sublattice magnetization is the same for all n considered ($n = 0$–4), indicating that the interchain quantum fluctuations affect only the overall magnitude of M. Hence even the conventional

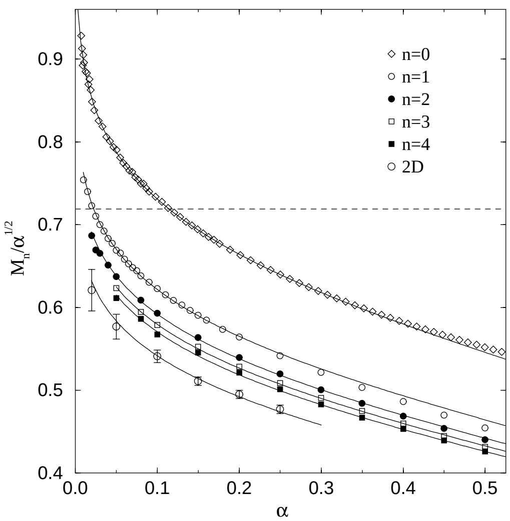

FIG. 2. Self-consistent staggered magnetization vs interchain coupling in the single-chain mean-field theory ($n = 0$) and multichain mean-field theories with $n = 1-4$. Statistical errors are at most comparable to the symbol sizes. Monte Carlo results for the full 2D Hamiltonian are shown with estimated error bars. The dashed line is the analytical $n = 0$ result [11]. The solid curves are of the form $M_n/\sqrt{\alpha} = A_n(1 + b\alpha)\ln^\gamma(a/\alpha)$, with $b = 0.095$, $a = 1.3$, and $\gamma = 1/3$ in all cases. These parameters, and $A_0 = 0.529$, were chosen to fit the $n = 0$ data. Only the amplitudes A_n were subsequently adjusted to fit the other data sets.

single-chain theory gives the correct functional form for M, although the magnitude is overestimated by a factor ≈1.35. The previous analytical treatment of the single-chain theory [11] misses the log correction.

For the model considered here, it was possible to explicitly test the multichain mean-field theory against large-scale quantum Monte Carlo results. In general, this would not be possible, e.g., for systems with frustrated interactions where Monte Carlo simulations suffer from sign problems. The density matrix renormalization group method [23] could be used to study the effective multichain models in such cases.

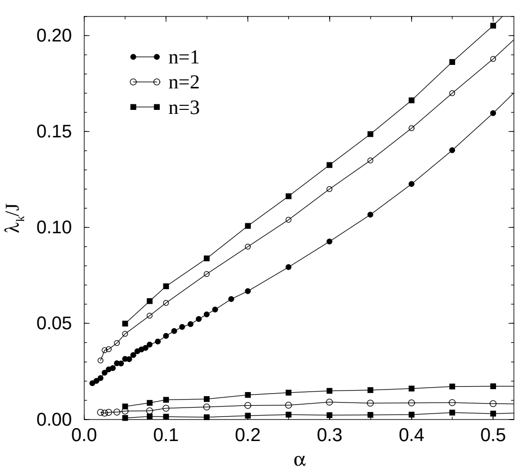

FIG. 3. Self-consistent anisotropy parameters vs interchain coupling for $n = 1, 2, 3$. All λ_k, $k = 1, \ldots, n$, for given n are shown using the same symbols, and in all cases $\lambda_1 < \cdots < \lambda_n$.

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Note added.—After completing this work, the author became aware of a recent bosonization calculation [24] predicting a log correction with exponent $\gamma = 1/2$ for M in the single-chain mean-field theory.

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