Multi-chain mean-field theory of quasi-one-dimensional quantum spin systems

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A multi-chain 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 neighbor chains \( C_\delta \), \( \delta = \pm 1, \ldots, \pm n \), 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 \( \alpha \) behaves as \( M \sim \sqrt{\alpha} \) enhanced by a multiplicative logarithmic correction.

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Quasi one-dimensional (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 \( t \) of the \( S = 1/2 \) Heisenberg chain has been observed in neutron scattering experiments on KCuF\(_3\) \( t \), and the Haldane gap predicted for integer \( S \) \( t \) has been detected, e.g., in the \( S = 1 \) compound CsNiCl\(_3\) \( t \). Quantum critical scaling \( t \) has been observed in the NMR relaxation rates of the \( S = 1/2 \) system Sr\(_2\)CuO\(_3\) \( t \), possibly even including anticipated \( s \) logarithmic corrections \( t \). 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\(_2\)CuO\(_3\) 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 cross-over 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 \( \delta \). The effective 1D system can be solved numerically on small lattices \( \delta \) or using analytical techniques \( \delta \). In this Letter, the mean-field approach is extended to include also a number of neighboring chains \( C_\delta \) 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 \( C_\delta \) 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 \( C_\delta \).

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

\[
H = J \sum_{i,j} S_{i,j} \cdot S_{i+1,j} + J_\perp \sum_{i,j} S_{i,j} \cdot S_{i,j+1},
\]

where \( S_{i,j} \) 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 \( M = \langle S_z^j \rangle \) 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 \( \alpha_c \) below which \( M = 0 \) \( t \), but RPA \( t \) gives \( \alpha_c = 0 \). Some self-consistent calculations predict \( \alpha_c \) \( t \) up to 0.2, whereas others have given \( \alpha_c \) as high as 0.8. Numerical simulations have not been presented; however \( \alpha_c = 0 \) appears most plausible \( t \). An analytical treatment of the single-chain mean field theory gave the behavior \( M \sim \sqrt{\alpha} \) for small \( \alpha \) \( t \). Numerically, \( M \) has been calculated using exact diagonalization \( t \) and series expansion techniques \( t \), the former indicating \( \alpha_c \approx 0.1 - 0.2 \), and the latter giving an upper bound \( \alpha_c \approx 0.02 \). Numerical calculations have in general been hampered by convergence problems and difficult extrapolations for small \( \alpha \). Here multi-chain mean-field calculations will be complemented by large-scale quantum Monte Carlo simulations of the original 2D Hamiltonian \( t \). It will be shown that quadratic lattices are not suitable for extrapolations to the thermodynamic limit when \( \alpha \ll 1 \), due to unusual, non-monotonic 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 \( \alpha \) 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 \( t \), the coupling of a chain \( j \) to its nearest-neighbors \( j \pm 1 \) is approximated by

\[
J_\perp \sum_i S_{i,j}^z (\langle S_{i,j-1}^z \rangle + \langle S_{i,j+1}^z \rangle)\]

In a Néel state \( \langle S_{i,j}^z \rangle = (-1)^{i+j} M \), and one obtains an effective 1D Hamiltonian,
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 multi-chain mean-field theory is to model the environment of a chain $C_0$ by its first few neighbor chains $C_\delta$, $\delta = \pm 1, \ldots, \pm n$, 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 $C_\delta$ chains should be considerably more realistic than just the static staggered field of the single-chain theory. If $C_0$ and $C_\delta$ 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 $C_\delta$. 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 $C_\delta$ is permissible). Here the simplest interaction satisfying this requirement will be considered, namely, the $xy$ part of the coupling is given a strength $J^\text{xy}_{\delta} = J(1 + \lambda_{\delta})$ different from $J^z_{\delta} = J$. Increasing $\lambda_{\delta} > 0$ increases the quantum fluctuations. The $(2n + 1)$-chain effective Hamiltonian is then

$$H_n = J \sum_{i=1}^{L} \sum_{j=-n}^{n} S_{i,j} \cdot S_{i+1,j} + J_\perp \sum_{i=1}^{L} \sum_{j=-n}^{n-1} S_{i,j} \cdot S_{i,j+1}$$

$$+ \sum_{i=1}^{L} \sum_{\delta=1}^{\delta=1} \sum_{\delta=1}^{\delta=1} \lambda_{\delta}(S_{i,\delta}^x S_{i+1,\delta}^x + S_{i,\delta}^y S_{i+1,\delta}^y)$$

$$+ h \sum_{i=1}^{L} (-1)^i(S_{i,-n}^z + S_{i,n}^z).$$

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

$$M \equiv M_0 = M_1 = \ldots = M_n,$$

$$h = MJ_\perp.$$

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 $0 < \lambda_1 < \ldots < \lambda_n$. For a given $\alpha$, 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 only affect the rate of convergence with increasing $n$.

Here quantum Monte Carlo results for the staggered structure factor on rectangular lattices with different aspect ratios and $\alpha = 0.05$. The behavior for a quadratic lattice with $\alpha = 0$ (independent 1D chains) is also shown. Statistical errors are much smaller than the symbols.
\( \beta = J/T \) as high as 2048 were used in order to obtain results free of temperature effects).

For \( \alpha = 1 \), the leading finite-size corrections to \( M^2 \) as defined in Eq. (2) are positive and \( \sim 1/\sqrt{N} \). This can be expected also for \( 0 < \alpha < 1 \) if the system is ordered. Fig. 2 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 \( \alpha_c \sim 0.1 - 0.2 \). Results for rectangular lattices with different aspect ratios \( R = L_x/L_y \) reveal a considerable dependence on \( R \), as also shown in Fig. 3. For \( R = 8 \), the expected linear behavior can be seen clearly, and for \( R = 4 \) there is a cross-over 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 non-monotonic, 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 non-monotonicity can be understood as resulting from a cross-over 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 \( \rho^2 \), then the system essentially behaves as a system of 1D chains, with exponentially damped correlations between the chains. A cross-over to 2D behavior can be expected when \( \Delta(L_x) \sim \rho^2 \), 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 \( \rho^2 < 1 \)), quadratic lattices therefore have to be very large for extrapolations to infinite size to be meaningful. Instead, rectangular lattices with \( R \) increasing with decreasing \( \alpha \) should be used. Using aspect ratios as large as \( R = 16 \), the sublattice magnetization was calculated for \( \alpha \) as small as 0.02. Below, the results will be compared with the single- and multi-chain 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 \( \mathcal{H} \). The effective model \( \mathcal{H} \) 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 \( \mathcal{H} \), the derivatives \( \partial M_j/\partial h \) and \( \partial M_j/\partial \lambda_k \) can also be calculated. Using these, an iterative scheme where

\[
\begin{align*}
\lambda_k(m+1) &= \lambda_k(m) + \Delta \lambda_k(m), \\
h(m+1) &= h(m) + \Delta h(m),
\end{align*}
\]

(7)

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

\[
\Delta h(0)(0) = \Delta \lambda_1(0)(0) = 0.
\]

FIG. 2. Self-consistent staggered magnetization vs inter-chain coupling in the single-chain mean-field theory (\( n = 0 \)) and multi-chain 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 \( A_n = 0.529 \), were chosen to fit the \( n = 0 \) data. Only the amplitudes \( A_n \) were subsequently adjusted to fit the other data sets.

\[
\begin{align*}
\Delta h(0)(0) &= \Delta \lambda_1(0)(0), \\
+\Delta \lambda_1(0)(0) &= \Delta M_1(0)/\partial h, \\
&= M_1 - M_0, \\
+\Delta \lambda_1(0)(0) &= \Delta M_1(0)/\partial \lambda_1 - \Delta M_1(0)/\partial \lambda_1 - M_1 - M_0, \\
&= 2h/J_\perp - M_1 - M_0.
\end{align*}
\]

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 \( \alpha \) 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 \( \mathcal{H} \), extrapolated to infinite size, are shown divided by \( \sqrt{\alpha} \) in Fig. 1. The behavior predicted by \( \mathcal{H} \) 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 \( \alpha < 0.4 \) is closely reproduced by the form \( M_0 = A_0\sqrt{\alpha}(1+b\alpha)\ln^\gamma(a/\alpha) \), with \( \gamma = 1/3 \), \( A_0 \approx 0.53 \), \( a \approx 1.3 \), and \( b \approx 0.1 \). This result shows that the mapping of Eq. (2) to the continuum model is

\[
\begin{align*}
\lambda(k) &= \lambda(k), \\
h(k) &= h(k) + \Delta h(k), \\
&= \lambda(k) + \Delta \lambda(k).
\end{align*}
\]
The behavior for \( n \) > 1, the anisotropy is always largest at the edges, as expected, and rapidly decreases as the center chain is approached. For \( \alpha \rightarrow 0 \), the 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 \( \alpha \rightarrow 0 \) suggests a very slow asymptotic decay to zero — again an indication of log-corrections.

To conclude, both the multi-chain 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. 2D quantum fluctuations develop systematically in the multi-chain theory as \( n \) is increased. For \( \alpha \ll 1 \), the functional form of the sublattice magnetization is the same for all \( n \) considered \( (n = 0 \rightarrow 4) \), indicating that the interchain quantum fluctuations only affect the over-all magnitude of \( M \). Hence even the conventional single-chain theory gives the correct functional form for \( M \), although the magnitude is over-estimated by a factor \( \approx 1.35 \). The previous analytical treatment of the single-chain theory \(^{[10]} \) misses the log-correction.

For the model considered here, it was possible to explicitly test the multi-chain 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 multi-chain models in such cases.

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\[ \lambda/J = 0 \ [22] \]

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