Thermodynamics of the One-Dimensional SU(4) Symmetric Spin-Orbital Model

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The ground-state properties and thermodynamics of the one-dimensional SU(4) symmetric spin system with orbital degeneracy are investigated using the quantum Monte Carlo loop algorithm. The spin-spin correlation functions exhibit a 4-site periodicity, and their low-temperature behavior is controlled by two correlation lengths that diverge like the inverse temperature, while the entropy is linear in temperature and its slope is consistent with three gapless modes of velocity $\pi/2$. The physical implications of these results are discussed. [S0031-9007(98)08155-1]

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In many transition metal oxides, the electron configuration has an orbital degeneracy in addition to the spin degeneracy. The sign and magnitude of the spin-spin interactions is then determined by the orbital occupation leading to strong coupling between orbital and spin structure (for an overview see Ref. [1]). The Hamiltonian describing such spin-1/2 systems with twofold orbital degeneracy (isospin $\tau = 1/2$) was derived by Kugel and Khomskii [2] and extensively studied in the context of V_2O_3 by Castellani *et al.* [3] more than 20 years ago. The Hamiltonian has rotation symmetry in $\vec{S}$ space. In $\vec{\tau}$ space this symmetry is broken by a Hund's rule term. Recently, the investigation of these spin-orbital models has attracted renewed interest, following the progress in the experimental studies of transition metal oxides [4–6].

In this Letter we study the Hamiltonian derived by Kugel and Khomskii on a 1D chain, but neglecting the Hund's rule term. In this isotropic case the Hamiltonian is

$$H = J \sum_i \left(2\vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{2}\right)\left(2\vec{\tau}_i \cdot \vec{\tau}_{i+1} + \frac{1}{2}\right). \quad (1)$$

It is rotationally invariant not only in $\vec{S}$ space, but also in $\vec{\tau}$ space. Furthermore it has an interchange symmetry between spins and orbitals. In such a case, the standard mean-field approach [3] that leads to ferromagnetic correlations for one type of variables and antiferromagnetic (AF) correlations for the other one should not be appropriate. Our main motivation is to study the consequences of this symmetry, in more detail.

A number of analytic results have already been obtained on this model. The system considered here [Eq. (1)], belongs to a class of models which is exactly solvable in one dimension by the Bethe ansatz. The Bethe ansatz solution obtained by Sutherland gives the exact ground-state energy and the "spin wave" excitations as well [7]. For the model of Eq. (1), there are 3 gapless modes, having all a common velocity $v = \pi J/2$. They are shown in Fig. 3 of Ref. [7].

Second, it was pointed out very recently [8,9] that the Hamiltonian H has not only the obvious SU(2) × SU(2) symmetry, but that the full symmetry of Eq. (1) is the even higher symmetry group SU(4). SU(N) symmetric models in one dimension were studied by Affleck, using conformal field theory [10]. He showed that any one-dimensional system of SU(N) symmetry is critical. He calculated explicitly the critical exponents and zero temperature correlations and showed that at the very low energy scale these models are equivalent to $N - 1$ free massless bosons. These general results naturally also apply to our case with $N = 4$.

In this Letter we present the first investigation of the thermodynamic properties of the model Eq. (1). For this purpose we have adapted the continuous time quantum Monte Carlo (QMC) loop algorithm [11] to spin-orbital models. For this kind of simulations three types of loop updates have to be included: Spin (orbital) loop updates, where only spin (orbital) variables are changed, but also spin/orbital loop updates where both spin and orbital are simultaneously updated. In fact, this algorithm is so powerful that we can also use it to investigate the zero-temperature properties of the model: Systems of length $L = 100$ [with periodic boundary conditions (PBC)] and inverse temperatures $\beta J = 400$ or 800 ($\beta \gg L/v$) are predominantly in the ground state, and the small contributions from thermally excited states are negligible compared to our statistical errors. In this way, the ground-state properties can be investigated. We start with a brief summary of these results since some of them differ significantly from the density matrix renormalization group (DMRG) results reported in Ref. [9].

The ground-state energy for a chain of $L = 100$ with periodic boundary condition is found to be $\epsilon_0(L = 100) = -0.8253(1)$, in perfect agreement with the Bethe ansatz result for the infinite chain ($-0.825\,118\,9\ldots$) [7]. The zero-temperature correlation function $w_{ij}(T = 0) \equiv \langle S_i^z S_j^z \rangle (T = 0)$ as a function of $|i - j|$ (for $L = 100$) is shown in Fig. 1a and its Fourier transform in Fig. 1b.

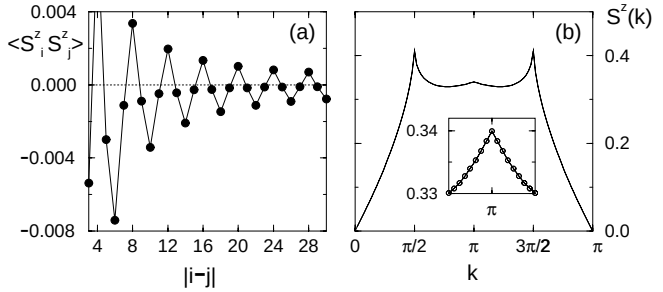

FIG. 1. (a) QMC results for the correlation function $w_{ij} \equiv \langle S_i^z S_j^z \rangle$ (solid points) as a function of $|i - j|$ for a chain of length $L = 100$ with PBC which is predominantly in the ground state (for details see text). The correlations for $|i - j| = 1$, 2, and 4 (which are out of the plot range) are $-0.071\,68(1)$, $-0.040\,11(1)$, and $0.008\,261(4)$, respectively. The statistical error bars of the QMC calculations are much smaller than the symbols. (b) shows the Fourier transform $S^z(k)$ of w_{ij} on two different scales.

Note that according to the SU(4) symmetry, all the following correlations are equal [8]:

$$\langle S_i^\alpha S_j^\alpha \rangle = \langle \tau_i^\alpha \tau_j^\alpha \rangle = \langle 4 S_i^\alpha S_j^\alpha \tau_i^\beta \tau_j^\beta \rangle = w_{ij}\,, \qquad (2)$$

independent of the indices α, $\beta = x, y, z$. This relation is valid for zero as well as for finite temperatures. While the first equality also holds for an arbitrary SU(2) $\times$ SU(2) symmetric model with exchange symmetry of the $\vec{S}$ and $\vec{\tau}$ variables, the second one is a special property of the SU(4) symmetric model. All the QMC results have been checked for the symmetry relation Eq. (2) and perfect agreement within the statistical error has been found.

The correlation function w_{ij} shows a clear 4-site periodicity (see Fig. 1). Its sign is positive if $|i - j| = 4N$, N integer and negative otherwise. The reason for the latter is the tendency for every four neighboring sites to form a SU(4) singlet [8]. Furthermore, from Fig. 1, it can be seen that the correlations for distances $|i - j| = 4N$ and $4N + 2$ decay much slower than for $|i - j| = 4N + 1$ and $4N + 3$. The explanation of this fact is simple: The system considered here has low-lying excitations at $k = 0$, $\pi/2$, and π (see Fig. 3 of [7]) each of them leading to a mode with wave vector k in the long distance correlations. The amplitudes of these modes are all expected to decay according to a power law, but with different critical exponents α_k. From the results for w_{ij} (Fig. 1), it can be concluded that the two dominant modes are those with $k = \pi/2$ (positive prefactor) and $k = 0$ (negative prefactor). This is also reflected in the Fourier transform $S^z(k)$ of the correlation function w_{ij}, having a characteristic cusp structure at $k = 0$, $\pi/2$, and π (see Fig. 1b). While the cusps at $k = 0$ and $\pi/2$ are quite sharp, the one at $k = \pi$, however, is not so pronounced, indicating that the $k = \pi$ mode is of all the three the least dominant mode in the correlation function.

The two critical exponents $\alpha_{\pi/2}$ and α_0 can be determined from the QMC data of the real space correlation function $w(r) \equiv w_{ij,|i-j|=r}$. Fitting $w(r)$ to the form $b_{\pi/2}[r^{-\alpha_{\pi/2}} + (L - r)^{-\alpha_{\pi/2}}]\cos(\frac{\pi}{2} r) + b_0[r^{-\alpha_0} + (L - r)^{-\alpha_0}]$ for the range $20 \lesssim r \lesssim 50$ (making explicit use that our system has PBC), we find

$$\alpha_{\pi/2} = 1.50 \pm 0.01, \qquad \alpha_0 = 1.85 \pm 0.16\,. \qquad (3)$$

The best fit is obtained for $b_{\pi/2} = 0.091$, $\alpha_{\pi/2} = 1.499$, $b_0 = -0.035$, and $\alpha_0 = 1.85$. A precise estimate of α_0 is not simple since the $k = 0$ mode is only a relative small superposition on the top of the much stronger $k = \pi/2$ mode. The exponent $\alpha_{\pi/2}$, however, can be determined to high precision. These results are in very good agreement with the prediction of Affleck, who calculated the critical behavior of the SU(4) correlation function in an arbitrary SU(4) symmetric model using conformal field theory [10]. This correlation function is proportional to w_{ij}, as a consequence of the symmetry relation Eq. (2) and the exact results are $\alpha_{\pi/2} = \frac{3}{2}$ and $\alpha_0 = 2$. The exponent $\alpha_{\pi/2}$ has also been estimated, using DMRG ($\alpha_{\pi/2} \simeq 1.5 \sim 2$) [9]. The DMRG results are in principle more precise than the QMC results, but finite size effects in DMRG studies are much bigger due to the use of open boundary conditions. Thus it is not surprising that our estimate Eq. (3) is much more precise.

At finite temperatures, the dominant components in the correlation function, $w_{ij}(T) \equiv \langle S_i^z S_j^z \rangle(T)$ [note that Eq. (2) holds also at finite T] which result from the soft modes at $k = 0$ and $\pi/2$, no longer decay according to a power law, but exponentially. The corresponding correlation lengths $\xi_0(T)$ and $\xi_{\pi/2}(T)$ may be different.

The correlation function $\langle S_i^z S_j^z \rangle(T)$ is shown as a function of $|i - j|$ in Fig. 2 for a system of length $L = 200$

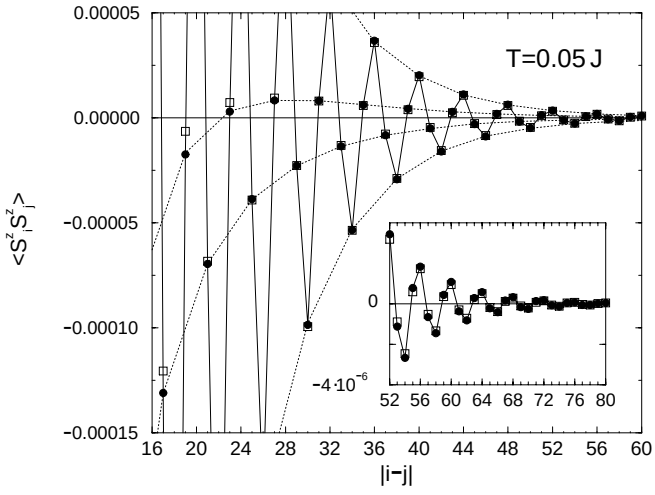

FIG. 2. QMC results for $w_{ij}(T) \equiv \langle S_i^z S_j^z \rangle(T)$ for a system of length $L = 200$ with PBC and at temperature $T = 0.05J$ (solid points). As a guide to the eye, the correlations at distances $|i - j| = 4N + m$ are connected by a separate (dotted) line for each $m = 0$, 1, 2, and 3. The inset shows the long distance correlations. The error bars are much smaller than the symbols. The open squares show the fit with Eq. (4).

with PBC at a temperature $T = 0.05J$. To find the correct low-temperature form, describing the long distance behavior ($|i - j| \gg \xi_0, \xi_{\pi/2}$) of the correlations $w_{ij}(T)$, one has to consider not only a phase shift $\delta(T)$ in the $k = \pi/2$ mode, but also an incommensuration effect of this component, i.e., that the period is shifted away from $k = \pi/2$ by an amount $\phi_k(T)$. This is due to the asymmetry of the excitation spectrum at the point $k = \pi/2$ which manifests itself at finite T, where also excited states contribute to $w_{ij}(T)$. This asymmetry can be seen in Fig. 2 of [9], where the degeneracy of the lowest spin wave branch is indicated. As the degeneracy for $k > \pi/2$ is larger than for $k < \pi/2$, we expect the weight of the $\pi/2$ mode to be shifted to a higher k value. This effect can also be observed in the Fourier transform $S^z(k, T)$ of the correlation function, where the maximum at $k = \pi/2$ at $T = 0$ moves to higher k values when T increases.

Finally, we propose the following low-temperature form for the correlations $w_{ij}(T)$ with $|i - j| \gg \xi_0, \xi_{\pi/2}$:

$$w_{ij}(T) = b_0(T)e^{-|i-j|/\xi_0(T)} + b_{\pi/2}(T)e^{-|i-j|/\xi_{\pi/2}(T)} \times \cos\{[\pi/2 + \phi_k(T)](i - j) + \delta(T)\}. \quad (4)$$

Fitting the above form to the QMC data of $w_{ij}(T)$ for various T gives the temperature dependence of the six parameters b_0, ξ_0, $b_{\pi/2}$, $\xi_{\pi/2}$, ϕ_k, and δ. The corresponding fit for $T = 0.05J$ is shown in Fig. 2. At this point, we want to emphasize that it is important to include the effect of incommensuration (i.e., including a parameter $\phi_k \neq 0$) to get accurate fits in the temperature range $0.01J \leq T \leq 0.08J$ and that at finite temperatures and larger distances, also the correlations at distances $4N + 3$ can become positive (Fig. 2), different from the correlations at $T = 0$. For all considered T, the correlation lengths are much smaller than the length of the system ($L > 6\xi_{\pi/2}, 6\xi_0$), so that finite size effects are negligible.

In Fig. 3 the inverse correlation lengths ξ_0^{-1} and $\xi_{\pi/2}^{-1}$ as well as the periodicity shift ϕ_k are plotted as a function of temperature. At very low temperatures, ξ_0^{-1} and $\xi_{\pi/2}^{-1}$ both show a linear behavior (see Fig. 3) and the leading temperature dependences are found to be

$$\xi_{\pi/2}^{-1} = (2.99 \pm 0.03)T, \qquad \xi_0^{-1} = (3.90 \pm 0.09)T. \quad (5)$$

Therefore both correlation lengths scale with $1/T$. This scaling behavior, including the prefactor, can be motivated in the following way. By the Lorentz invariance of the underlying field theory of the considered model and by exchange of the imaginary time and space direction, one has $\xi_k(T) = v/\Delta_k(L = v/T)$, where $\Delta_k(L)$ is the finite size gap to the lowest excitations at wave vectors $\approx k$ in a system of length L. v is the spinon velocity, which in our model is $\pi J/2$. For $k \approx 0$, the lowest lying excitation energy is $\Delta_0(L) = v(2\pi/L)$ leading to $\xi_0 = J/(4T)$, in good agreement with Eq. (5). For $k = \pi/2$, the finite size results of Ref. [9] show that $\Delta_{\pi/2}(L) \approx 0.75\Delta_0(L)$ (a similar result should be obtained, using field theory) and hence $\xi_{\pi/2} \approx J/(3T)$, again in very good agreement with Eq. (5). In comparison, the leading temperature dependence of the correlation length in the SU(2) AF Heisenberg model [$H_{\mathrm{HB}} = J\sum_i \vec{S}_i \cdot \vec{S}_{i+1}$, $v_{\mathrm{HB}} = \pi J/2$, and $\Delta_\pi^{\mathrm{HB}}(L) = \pi v/L$] is $\xi_\pi^{\mathrm{HB}}(T) = J/(2T)$.

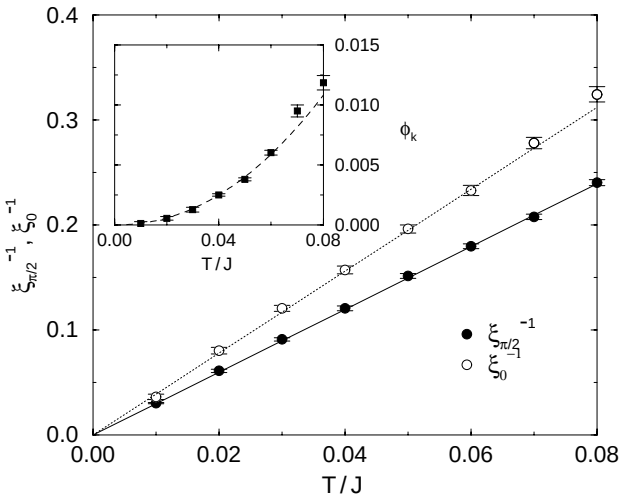

FIG. 3. Inverse correlation lengths ξ_0^{-1} (open circles) and $\xi_{\pi/2}^{-1}$ (filled circles) and the periodicity shift ϕ_k (inset) as a function of temperature. The leading T dependences [Eq. (5)] are also shown (solid, dotted, and dashed lines).

The leading T dependence of the periodicity shift ϕ_k has been obtained by fitting the very low-temperature data with λT^β, and the result is $\phi_k(T) \propto T^{2.11\pm0.15}$. This scaling exponent is quite close to the value of 2, which one would expect from a simple calculation, considering the thermal admixtures of the spin wave branches.

Finally, we concentrate on the entropy s per site of the SU(4) invariant model of Eq. (1). Its T dependence $s(T)$ is shown in Fig. 4. With decreasing T, the entropy decreases monotonically from the high-temperature value $\ln 4$ to 0 at zero temperature. At low temperatures the entropy shows a linear behavior as in the AF SU(2) Heisenberg chain (H_{HB}). The slope in the spin-orbital model, however, is about a factor of 3 bigger than that in the AF Heisenberg chain (see inset of Fig. 4). This is consistent with the statement of Affleck [10] that the AF Heisenberg model is equivalent to *one* free massless boson, while the SU(4) invariant spin-orbital model is equivalent to *three* massless bosons. The velocity of these bosons are all equal to $\pi J/2$ [7,12]. Therefore we expect the low energy density of states (and hence the entropy) of these two models just to differ by a factor of 3.

The implications of these results for mean-field treatments are far reaching. To put them in perspective, it is useful to compare them to the standard mean-field decoupling [3] $(\vec{S}_i \cdot \vec{S}_{i+1})(\vec{\tau}_i \cdot \vec{\tau}_{i+1}) \rightarrow \langle \vec{S}_i \cdot \vec{S}_{i+1}\rangle \vec{\tau}_i \cdot \vec{\tau}_{i+1} + \langle \vec{\tau}_i \cdot \vec{\tau}_{i+1}\rangle \vec{S}_i \cdot \vec{S}_{i+1} - \langle \vec{S}_i \cdot \vec{S}_{i+1}\rangle \langle \vec{\tau}_i \cdot \vec{\tau}_{i+1}\rangle$. Such a decoupling has a number of consequences. First of all,

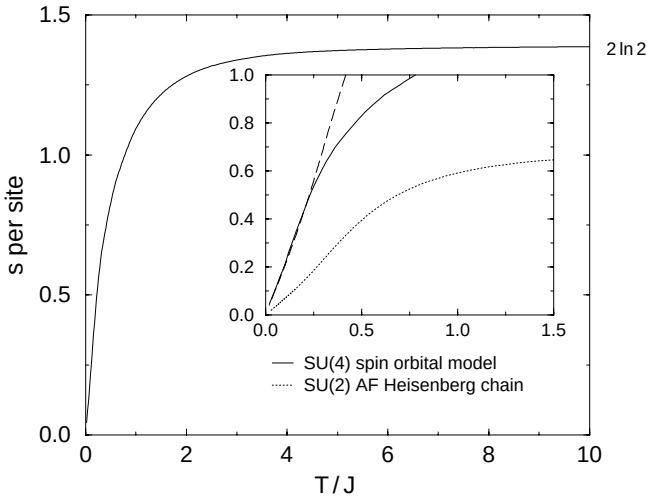

FIG. 4. Temperature dependence of the entropy s per site for the spin-orbital model Eq. (1) (solid line). In the inset the entropy per site is shown on larger temperature scale together with the entropy s_{HB} per site of a SU(2) spin-1/2 AF Heisenberg chain (H_{HB}) (dotted line). For comparison also $3s_{\mathrm{HB}}$ is shown (dashed line).

the correlation function $\langle(\vec{S}_i \cdot \vec{S}_{i+1})\,(\vec{\tau}_i \cdot \vec{\tau}_{i+1})\rangle$ should be equal to the product of $\langle\vec{S}_i \cdot \vec{S}_{i+1}\rangle$ with $\langle\vec{\tau}_i \cdot \vec{\tau}_{i+1}\rangle$, in clear contradiction both with the fact that all of them are negative according to our results and with the property of Eq. (2). Besides, and more importantly, if such a decoupling was a valid approximation, the low-lying excitations should consist of two branches corresponding to spin and orbital excitations, respectively. This is again in clear contradiction with the three low-lying modes of the Bethe ansatz which control the low-temperature physics according to our entropy results. So there is a manifest breakdown of the mean-field decoupling when spin and orbital degrees of freedom play a symmetric role.

What is then the nature of the low-lying excitations? A full answer cannot be given on the basis of the present results, but a number of conclusions can be reached. Let us start with the 2-site problem. The ground state is sixfold degenerate (spin-triplet $\times$ orbital-singlet or spin-singlet $\times$ orbital-triplet), and energy may be gained by allowing fluctuations between these local configurations. The mean-field decoupling fails because it cannot take advantage of these fluctuations. Elementary considerations show that the best mean-field decoupling leads to a very poor estimate of the ground-state energy (-0.3863 vs -0.8251 for the exact result). That it is possible to gain energy by allowing the system to fluctuate locally is best exemplified by the 4-site problem. In fact, the exact ground state for a 4-site cluster with periodic or open boundary conditions, the SU(4) singlet of Ref. [8], can be obtained exactly in terms of these dimer wave functions, and the energy per bond is equal to -1; i.e., each bond has now managed to reach its ground-state energy thanks to the fluctuations between these six local configurations. Note that this is no longer true for longer systems, indicating that 4-site clusters should be a good starting point for building variational wave functions. This can be seen as the physical origin of the 4-site periodicity of the correlation functions. A similar conclusion was reached in Ref. [8] on the basis of the SU(4) symmetry.

Finally, if the ground state is a resonating-valence-bond-like state involving resonances between different local configurations, we are led to the conclusion that the elementary excitations cannot be pure spin or orbital excitations, but composite objects where spin and orbital degrees of freedom are intimately mixed. Work is in progress to get a more precise picture of these excitations. In addition, the presented results will also have dramatic consequences for more realistic models where the interchange symmetry between spin and orbital degrees of freedom is only approximately valid. This is left for future investigation.

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