Monte Carlo study of a one-dimensional degenerate Hubbard model

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(Received 20 May 1986; revised manuscript received 16 September 1986)

Correlations of a one-dimensional doubly degenerate Hubbard model are studied for the one-quarter-filled case. Exact calculations on a four-site lattice show that a ferromagnetic state exists in the strong-coupling regime. For a one-dimensional chain, a strong-coupling effective Hamiltonian was studied using a self-consistent calculation, a high-temperature expansion, and quantum Monte Carlo simulations. The results provide information on the parameters needed for ferromagnetic correlations, and the temperature dependence of the spin and orbital correlations.

In an early study of itinerate ferromagnetism, Slater, Slatz, and Koster[1] investigated the problem of two electrons on a one-dimensional lattice with nearest-neighbor hopping and onsite Coulomb interactions. For a nondegenerate band, they found that the ground state for the two particles was a singlet. However, for a narrow degenerate band in the strong coupling regime where the ratio for the Coulomb interaction strength to bandwidth is large, they showed that the ground state of the two-particle system was a triplet. This was in agreement with Van Vleck's suggestion[2] that the intra-atomic exchange interaction between electrons in degenerate orbitals, Hund's rule, was an important mechanism for itinerate ferromagnetism. However, the relationship of the two-electron problem to the many electron problem remained an open question and has subsequently been investigated using a variety of approximate techniques. Roth[3] examined the doubly degenerate, three-dimensional one-quarter-filled case in which there is one electron per site. In the narrow-band limit Roth assumed that the ground-state spins line up ferromagnetically as suggested by Van Vleck[2] and used the random-phase approximation (RPA) to investigate the spin-wave spectrum and the stability of the ferromagnetic state. She also found that the system formed an orbital superlattice structure in which the lattice orders into two sublattices distinguished by the occupation of different orbital states. Kugel and Khomskii[4] and Cyrot and Lyon-Caen[5] constructed a strong-coupling effective Hamiltonian and discussed the orbital superlattice and ferromagnetic transition using a Hartree-Fock approximation. Torrance[6] has suggested that a quasi-one-dimensional ferromagnetic system could be obtained from homogeneous stacks of double degenerate molecules in the strong-coupling limit. These results show that a natural generalization of ordinary superexchange[7] in the case of orbital degeneracy leads not only to magnetic ordering, but also to orbital ordering. With the current effort to synthesize quasi-one-dimensional ferromagnetic materials,[8] it is of interest to return to the orbitally degenerate quasi-one-dimensional model originally studied in Ref. 1 and examine its properties when many electrons are present.[9]

The model has the following form[10]

$$H=\sum_{i,\lambda,s}-t(d^{+}_{i+1,\lambda,s}d_{i,\lambda,s}+\text{h.c.})+\sum_{i,\lambda}Un_{i,\lambda,\uparrow}n_{i,\lambda,\downarrow}+\sum_{i,s,s'}Vn_{i,1,s}n_{i,2,s'}-\sum_{i,s,s'}Jd^{+}_{i,1,s}d_{i,2,s'}d^{+}_{i,2,s'}d_{i,2s}\ , \tag{1}$$

where the operator $d_{i,\lambda,s}$ is an annihilation operator for a Wannier electron at the site i, in the λ orbital ($\lambda=1,2$) with spin s. The parameter t is a hopping integral between nearest-neighbor sites, and we assumed that the two λ orbitals are not mixed by the hopping. The second term, proportional to U, represents the intraorbital Coulomb repulsion. The third term, proportional to V, describes the interorbital Coulomb repulsion and the final term containing J represents the exchange interaction, or, Hund's rule coupling. From now on, we will consider the one-quarter-filled case such that the average electron density per site is one.

For small lattices, H can be directly diagonalized. The phase diagram of the four site system with four electrons is shown in Fig. 1. Here we set the intraorbital Coulomb

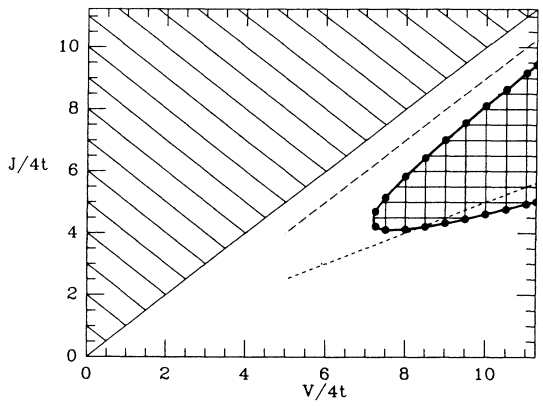

FIG. 1. Ground-state phase diagram of the four-site system with $U=V+J$. Since J is smaller than the Coulomb repulsion V, the physical regime lays below the diagonally shaded area. In the cross hatched region the ground state is fully spin aligned with $S=2$. Approximate lower $J=(\sqrt{2}-1)V$ and upper ($J=V-4t$) phase boundaries are shown by the short and long dashed lines, respectively.

repulsion U equal to $V+J$ preserving the rotational symmetry. One clearly sees that the ferromagnetic regime occurs when Coulomb repulsions and the exchange interaction are large compared with the bandwidth. Some physical insight regarding the phase boundaries can be obtained by examining various competing effects in the strong-coupling limit. The lower boundary of the ferromagnetic ($S=2$) regime arises from the competition between the usual antiferromagnetic superexchange[7] $\sim t^2/U$ and the ferromagnetic direct exchange[7] $\sim t^2J/(V^2-VJ)$. Equating these energies for $U=V+J$ gives the short dashed line $J=(\sqrt{2}-1)V$ in Fig. 1, which forms an approximate lower ferromagnetic phase boundary. The upper boundary arises from the competition between the hopping t and the energy $V-J$ which favors the orbital superlattice. When $V-J\lesssim 4t$ the orbital superlattice structure breaks down. The electrons lose their localized character, and a coherent singlet state becomes lower in energy than the magnetic ($S=2$) state. In Fig. 1, the long dashed line $J=V-4t$ gives the approximate upper bound.

From this four-site study, we clearly see that the phase boundary is in the strong-coupling regime. Therefore, it is useful for the one-dimensional problem to make a strong-coupling expansion leading to an effective Hamiltonian,[4,5]

$$\begin{aligned} H_{\text{eff}}=&\sum_i \frac{8t^2}{U}(\mathbf{S}_i\cdot\mathbf{S}_{i+1}-\tfrac{1}{4})(L_i^zL_{i+1}^z+\tfrac{1}{4}) \\ &+\frac{4t^2}{V-J}(\mathbf{S}_i\cdot\mathbf{S}_{i+1}+\tfrac{3}{4})(\mathbf{L}_i\cdot\mathbf{L}_{i+1}-\tfrac{1}{4}) \\ &-\frac{4t^2}{V+J}(\mathbf{S}_i\cdot\mathbf{S}_{i+1}-\tfrac{1}{4})[L_i^zL_{i+1}^z-\tfrac{1}{4}-\tfrac{1}{2} \\ &\times(L_i^+L_{i+1}^-+L_i^-L_{i+1}^+)] . \end{aligned} \tag{2}$$

Here S is the usual spin-$\frac{1}{2}$ operator and L is a "pseudo" spin-$\frac{1}{2}$ operator which describes the orbital state with $L_z=\frac{1}{2}$ and $-\frac{1}{2}$ corresponding to $\lambda=1$ and 2, respectively. We are interested in the zero-frequency q-dependent spin and orbital susceptibilities

$$\begin{aligned} \chi_s(q)&=\frac{1}{N}\sum_{i,l} e^{iql}\int_0^\beta d\tau\langle S_{i+l}^z(\tau)S_i^z(0)\rangle , \\ \chi_L(q)&=\frac{1}{N}\sum_{i,l} e^{iql}\int_0^\beta d\tau\langle L_{i+l}^z(\tau)L_i^z(0)\rangle . \end{aligned} \tag{3}$$

At low temperatures, in the (J,V,U) parameter regime where ferromagnetic correlations are present, it is useful to approximate $\mathbf{S}_i\cdot\mathbf{S}_{i+1}$ by $\langle\mathbf{S}_i\cdot\mathbf{S}_{i+1}\rangle$ leading to a quantum spin-$\frac{1}{2}$ Hamiltonian for the orbital degrees of freedom

$$H_L=\sum J_L(L_i^+L_{i+1}^-+L_i^-L_{i+1}^++\lambda L_i^zL_{i+1}^z) \tag{4a}$$

with J_L and λ depending on $\langle\mathbf{S}_i\cdot\mathbf{S}_{i+1}\rangle$ according to Eq. (2). Similarly, replacing the $\mathbf{L}_i\cdot\mathbf{L}_{i+1}$ operators in Eq. (2) by $\langle\mathbf{L}_i\cdot\mathbf{L}_{i+1}\rangle$, one obtains

$$H_s=\sum 2J_s\mathbf{S}_i\cdot\mathbf{S}_{i+1} \tag{4b}$$

with J_s depending on the various $\langle\mathbf{L}_i\cdot\mathbf{L}_{i+1}\rangle$ expectation values of Eq. (2). It is straightforward to carry out Monte Carlo simulations[11,12] of the XXZ models described by Eqs. (4) and to self-consistently solve them obtaining $J_L(T)$, $\lambda(T)$, and $J_s(T)$ as well as the correlation functions $\chi_s(q,T)$ and $\chi_L(q,T)$. Note that while H_s is isotropic, λ in H_L depends on U, V, and J. As T decreases, the self-consistent solution for λ approaches[13] the isotropic limit 2. Figure 2 shows $\chi_s(q=0)$ in the ferromagnetic regime verses β for various J/V and U/V values. Throughout this work we measure T in units of rt^2/V and have multiplied the susceptibilities by this same factor to make them dimensionless. As seen in Fig. 2, $\chi_s(q=0)$ is enhanced when J is increased, but is relatively independent of U when U is large. For $U=\infty$, $\chi_s(q=0)$ and $\chi_L(q=\pi)$ are shown as the solid lines in Figs. 3(a) and 3(b). The dashed lines are obtained from the $U\to\infty$ limit of the high-temperature series expansions,[14]

$$\frac{\chi_s(q=0)}{\beta}=\frac{1}{4}\left[1+\frac{\beta t^2J}{V^2-J^2}+\frac{3\beta^2t^4VJ}{(V^2-J^2)^2}\right] , \tag{5}$$

$$\frac{\chi_L(q=\pi)}{\beta}=\frac{1}{4}\left[1+\frac{\beta t^2(2V+J)}{V^2-J^2}+\frac{4\beta t^4(V^2+VJ+J^2)}{3(V^2-J^2)^2}\right] .$$

As first discussed by Roth,[3] the staggered orbital susceptibility $\chi_L(q=\pi)$ shows a clear indication of the formation of superlattice correlations in which alternate degenerate orbitals $\lambda=1$, $\lambda=1$ are occupied as T decreases. In such a system there will be a natural tendency to dimerize. In this work we have focused on the electronic correlations on a rigid lattice. Extensions of this approach to a dynamic lattice will be interesting.

In order to further test the high- and low-temperature approximations, a Monte Carlo simulation of H_{eff}, Eq. (2), with $U=\infty$ was carried out. The world line method[11] we used treats a restricted ensemble in which all

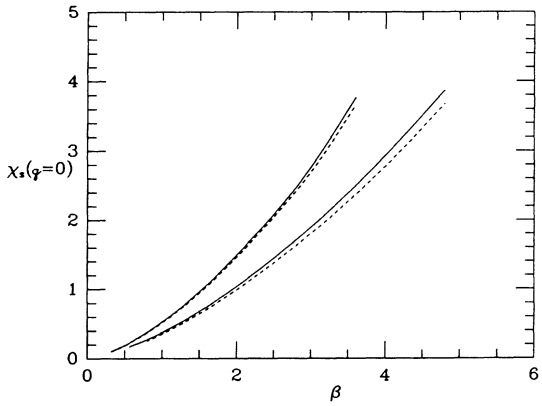

FIG. 2. $\chi_s(q=0)$, obtained from the low-temperature self-consistent approximation versus the inverse temperature $\beta=1/T$. The upper two and lower two curves correspond to $J/V=0.75$ and $J/V=0.5$, respectively. The solid and dashed lines correspond to $U/V=\infty$ and $U/V=1+J/V$, respectively.

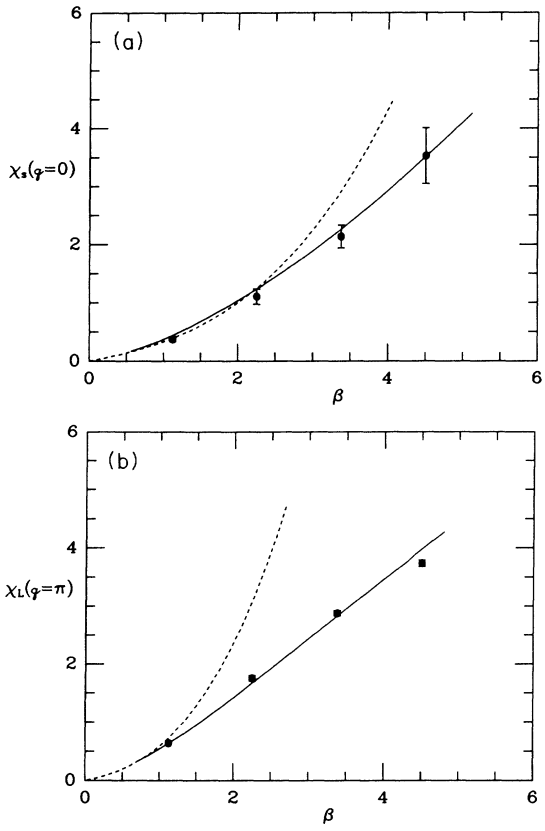

FIG. 3. (a) $\chi_s(q=0)$ and (b) $\chi_L(q=\pi)$ versus β, with T for $U=\infty$ and $J/V=0.5$. The solid curves are the self-consistent approximation, the dashed curves are the high-temperature expansion, Eq. (5), and the points are Monte Carlo data for a 20-site lattice.

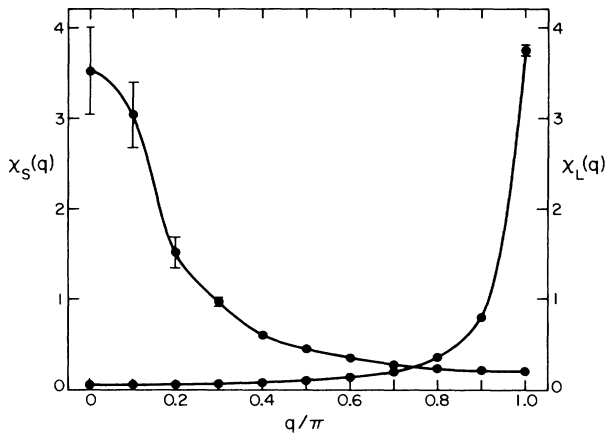

FIG. 4. $\chi_s(q)$ and $\chi_L(q)$ versus q for the same parameters as Fig. 3 and $\beta=4.5$. Circles are Monte Carlo results on a 20-site lattice, and the solid lines are a guide to the eye.

configurations have a total z component of spin equal to zero. In the thermodynamic limit, the physical results obtained from such a restricted ensemble will be the same as those from a nonrestricted ensemble. For finite systems, however, care must be taken to calculate appropriate physical quantities. For example, the $q=0$ susceptibilities are obtained by extrapolating the finite q-dependence of $\chi(q)$. Results for the q-dependent spin and orbital susceptibilities on a 20-site lattice are shown in Fig. 4. The low-momentum peak in χ_s clearly indicates the formation of ferromagnetic spin correlations. Similarly, the peak in the orbital susceptibility at $q=\pi$ implies that the system has a tendency for alternate orbitals to be occupied.[3] The peak values $\chi_s(q=0,\beta)$ and $\chi_L(q=\pi,\beta)$ obtained from Monte Carlo simulations of H_{eff} at different temperatures are shown as points with error bars in Figs. 3(a) and (b).

This analysis has provided detailed information on the many-electron (one-quarter-filled) one-dimensional doubly degenerate Hubbard model. In the strong coupling regime, the intra-atomic exchange interaction leads to long wavelength ferromagnetic and "staggered" orbital correlations. The Monte Carlo calculations along with the high- and low-temperature approximations provide a description of the temperature dependence of these spin and orbital correlations. From the full Monte Carlo calculation of the strong coupling Hamiltonian, Eq. (2), it appears that the simpler self-consistent solution, which involves only the simulation of the XXZ model, Eqs. (4), provides a useful approximation when ferromagnetic correlations are present.

We would like to acknowledge useful discussions with J. Bardeen, P. Grant, J. Hirsch, and H.-B. Schüttler and to thank M. Jarrell for help with the XXZ model. We also thank J. Miller, J. Torrance, and F. Wudl for discussions of these ideas and their possible application to new materials. This work was supported by the National Science Foundation under Grant No. DMR83-20481. One of us (D.J.S.) would also like to acknowledge support by the National Science Foundation under Grant No. Phy82-17853, supplemented by funds from the National Aeronautics and Space Administration.

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