Critical Properties of a Spin-$\frac{1}{2}$ Chain with Competing Interactions

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The crossover between $2k_F$ and $4k_F$ charge-density waves in an extended one-dimensional Hubbard model is studied in the $U\rightarrow\infty$ limit by mapping onto a Heisenberg antiferromagnet with a competing second-neighbor Ising interaction. The phase diagram is obtained by a combination of field-theory techniques and numerical solution of finite chains. Regions of staggered spin order ($4k_F$ site or bond order) and (2,2) spin order ($2k_F$ site order) are mapped out. Critical exponents in the algebraic phase are obtained.

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A number of models of interest in statistical mechanics, field theory, and the many-body problem are related to the spin chain

$$\mathcal{H}=\sum_n -\{J_x(S_n^xS_{n+1}^x+S_n^yS_{n+1}^y) +J_1S_n^zS_{n+1}^z+J_2S_n^zS_{n+2}^z+HS_n^z\}, \quad (1)$$

where S_n^x, S_n^y, and S_n^z are Pauli matrices. There is particular interest in the case of antiferromagnetic coupling ($J_1,J_2>0$) for which the competition between first- and second-neighbor exchange gives rise to a rather rich variety of physical behavior. Equation (1) is a generalization of the XXZ model[1] and the lattice Hamiltonian versions of the Thirring[2] and Van Beijeren[3] models. It may be compared to the Hamiltonian form of the anisotropic next-nearest-neighbor Ising model[4] in which the spin-flip term is replaced by $J_x\sum S_n^x$. But our main interest is to use $\mathcal{H}$ as a model for the so-called $2k_F$ and $4k_F$ charge-density-wave (CDW) instabilities in organic conductors,[5] making use of the exact mapping[6] between $\mathcal{H}$ and the extended Hubbard model with infinite on-site interaction U. In this representation, S_n^z is $+1$ if a site is occupied by an electron and -1 if it is unoccupied, J_x is the transfer integral, J_1 and J_2 are Coulomb interactions, and H is the chemical potential. Scattering experiments[5] have found evidence for two kinds of CDW in organic conductors, one of which is thought to be related to a Peierls transition and the other to the formation of a Wigner crystal. Although some materials display both CDW's, there is little understanding of the crossover from one to the other as parameters such as the temperature and pressure are varied. This is what we hope to attain by a study of the spin chain for which the CDW's correspond to various forms of magnetic order.

Hirsch and Scalapino[7] have used a quantum Monte Carlo method to study CDW's in the extended Hubbard model with $J_2=0$ and U infinite. We shall use a different approach to show how the inclusion of second-neighbor interactions, which is reasonable on physical grounds, gives rise to a significant modification of the behavior. The use of spin representation gives a particularly clear interpretation of the phase diagram and also leads to results of interest for spin chains in general.

The ground state of $\mathcal{H}$ is known for certain limiting values of the parameters. When $J_x=0$, the Hamiltonian is a simple Ising mode whose ground state (for $H=0$) is antiferromagnetic (AF) for $J_1<2J_2$ and a (2,2) state $(++--++--\cdots)$ otherwise. In electron-gas language they correspond to the Wigner crystal and Peierls CDW, respectively. The ground state at $J_1=2J_2$ is highly degenerate. On the other hand, when $J_2=0$ but J_x is finite, exact results[1] show that the AF order persists up to $J_x=J_1$ where it gives way to an algebraic phase with power-law correlation functions.

Figure 1 shows the more general phase diagram which we have established for $H=0$ (zero magnetization or a quarter-filled band in the Hubbard model). The algebraic region is a plane of critical points whose exponents are functions of a single variable $\theta(J_x/J_1,J_2/J_1)$. It will be seen that this phase is best characterized by the θ contours, and that $\theta=1$ is the boundary between algebraic and ordered phases shown in Fig. 1. The latter have either AF order or staggered order in the XY spin plane [which will be shown to be equivalent to bond order (BO) in electron-gas language], separated by a line of fixed points shown as the broken line in Fig. 1. The (2,2) order appears through an additional transition within the BO region, and it competes with the BO, finally destroying it at $J_x=0$.

Since an exact solution is not available for $J_2\neq0$, we have obtained these results by using a combination of analytical and numerical methods to relate the lattice model to a continuum field theory from which the asymptotic behavior of the correlation functions may be obtained. The essence of the method is as follows. If $\mathcal{H}$ is rewritten in terms of fermion variables,[6] it contains both direct and umklapp scattering processes[8-10] with coupling constants g_d and g_u, respectively. For weak

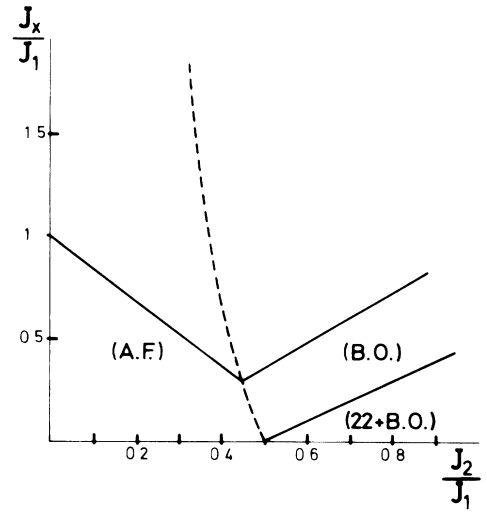

FIG. 1. Phase diagram for the model. The ordered phases are antiferromagnetic (AF), bond ordered (BO), and (2,2) as described in the text. They correspond to $4k_F$ site order, $4k_F$ bond order, and $2k_F$ site order, respectively. The region above the ordered phases is a plane of critical points. The broken line is a line of fixed points of the renormalization-group equations (2). It is stable in the algebraic region and unstable between the ordered phases.

coupling $(g_d,g_u)\sim(J_1,J_1-4J_2)$. In writing down the renormalization-group (RG) equations which govern the approach to the continuum limit, it is best to change variables from (g_d,g_u) to (θ,g_u) so that the variable θ, defined above, appears directly. If we denote the renormalized values of θ and g_u by $\bar{\theta}$ and $\bar{g}_u$, the RG equations to lowest order in $\bar{g}_u$ are[9]

$$d\bar{\theta}/dl = a\bar{g}_u^2, \tag{2a}$$

$$d\bar{g}_u/dl = (2-2/\bar{\theta})\bar{g}_u, \tag{2b}$$

where l is the logarithm of a cutoff, to be specified later. Long-range order is produced when $\bar{g}_u$ is a relevant variable as l increases; otherwise the correlation functions are power laws.[8-10] With use of Eq. (2b) this means that the phase boundary occurs when $\theta=1$, where θ is the value of $\bar{\theta}$ at $\bar{g}_u=0$.

In order to use this result to determine the phase boundaries shown in Fig. 1 and to evaluate θ in the algebraic phase, it is necessary to carry out the global renormalization from the original model, where $\bar{g}_u$ may not be small, to the neighborhood of the fixed line, $\bar{g}_u=0$, where Eqs. (2) are valid. For $J_2=0$, Luther and Peschel[11] made use of known critical exponents[1] to show that $\cos\pi\theta=-J_1/J_x$. For the general case it is necessary to use numerical methods.

As a controlled approximation, we have diagonalized the Hamiltonian $\mathcal{H}_N$ for N sites on a ring in order to obtain boundary conditions for the RG equations (2), using $l\equiv\ln N$. This approach has a greater analytical input than the usual finite-size scaling method and can give a much higher accuracy. The idea is to identify the size dependence of $\bar{g}_u$ through its effect on the energy levels of $\mathcal{H}_N$, as used in a related study of the Potts models.[9] For $J_1=0=J_2$, the fermion form of $\mathcal{H}$ may be diagonalized to give a cosine band which is half-filled and has Fermi surface $k_F=\pm\pi/2$ when $H=0$. For fixed particle number, the lowest excited levels $|A\rangle$ and $|B\rangle$ with energies E_A and E_B have momenta $\pm\pi$ and are produced by the transfer of a particle to the left or the right across the Fermi surface. In the absence of interactions, $E_A=E_B$, but in general the states are coupled by umklapp scattering and the level splitting E_A-E_B gives a measure of $\bar{g}_u$. Equations (2) sum all orders of perturbation theory to produce an effective interaction $\bar{g}_u$ (dependent on N) from which E_A-E_B may be evaluated in first-order degenerate perturbation theory. The analysis involves two steps: (i) Determine $\bar{g}_u(N)$ numerically and use it to find $\bar{\theta}(N)$ from the discrete form of Eq. (2b),

$$\Delta\ln\bar{g}_u=(2-2/\bar{\theta})\Delta\ln N; \tag{3}$$

(ii) fit the results to the solution of Eqs. (2),

$$A\bar{g}_u^2=\bar{\theta}-\theta-\ln(\bar{\theta}/\theta), \tag{4}$$

in order to determine the constants of integration A and θ. Then θ is the value of $\bar{\theta}$ on the fixed line $\bar{g}_u=0$, as required. The accuracy of this procedure is illustrated in Table I by a comparison with the known exact values of θ for $J_2=0$. Usually it is not easy to obtain accurate values of critical exponents in regions where there are two marginal variables, and the good agreement we have obtained reflects the full utilization of the information contained in the RG equations.

TABLE I. Critical exponent parameter for $J_2=0$. Values obtained from the renormalization-group method (RG) described in the text and from Luck's relation are compared to the known analytical values.

J_x/J_1	RG	Luck's relation	Exact
1	0.953	0.995	1.0
1.25	0.796	0.814	0.795
1.50	0.734	0.733	0.732
1.75	0.696	0.694	0.694

But the analysis is not so straightforward everywhere. In lowest order, $g_u\sim J_1-4J_2$ and the levels E_A and E_B cross when $J_2=J_1/4$. As J_x is decreased, the degeneracy point traces out a line which generally depends upon N but passes through $J_2=J_1/2$ as $J_1/J_x\to\infty$. For $N\to\infty$ this is in fact the fixed line of Eqs. (2) just as the θ contours are the flow lines. The phase diagram of Fig. 1 is then an image of the full RG flows. However, it is clear that when the size dependence of E_A-E_B is significantly affected by the movement of the fixed line with N, it cannot simply be used a means of determining θ, and it is

necessary to find some other method. We have chosen to use Luck's relation[12] for the splitting Δ_N between the ground and first excited states of an N-site system:

$$N\Delta_N = \pi v_F/\theta, \tag{5}$$

where v_F is the Fermi velocity.[13] Table I illustrates the accuracy of the method for $J_2=0$. To obtain Fig. 1, Eq. (5) was used in the algebraic region for $0.2 < J_2/J_1 < 0.7$, which allowed a sufficient overlap with the other methods of determining θ and the phase boundary.

Turning now to discussion of the ordered regions, it is expected that the AF phase, which is known to exist for $J_2=0$, should extend out to finite values of J_2 but change its character across the fixed line. This may be understood by our carrying out a chiral transformation[14] which reverses the sign of $\bar{g}_u$ and effects the following change in the staggered magnetization operator:

$$\sum_m (S^z_{2m} - S^z_{2m+1}) \rightarrow \sum_m (S^x_{2m}S^x_{2m+1} + S^y_{2m}S^y_{2m+1}). \tag{6}$$

Then the right-hand side of (6) should give the order parameter on the large-J_2 side of the fixed line. This is a staggered order in the XY plane or bond order in electron-gas language, since it is a staggered kinetic energy in the fermion representation. As noted by Haldane,[15] the existence of the BO phase is also suggested by comparison with another, exactly solved, second-neighbor model,[16] which lies in the $g_u < 0$ sector and has a dimerized ground state equivalent to a fully saturated BO parameter. However, this cannot be the whole story for the Hamiltonian of Eq. (1): There must be a further transition to establish the (2,2) order which we know to exist at $J_x=0$. We have verified this picture and obtained the phase assignments of Fig. 1 by evaluating the order parameters numerically and extrapolating to $N \rightarrow \infty$ in the manner of Bonner and Fisher.[17]

It is possible to give a more detailed account of the competition between BO and (2,2) order. In the AF and BO phases of the infinite system, the lower of the two states $|A\rangle$ and $|B\rangle$ is degenerate with the ground state, and there are two equivalent phases related by displacement through one lattice site. But the (2,2) phase is fourfold degenerate. The two additional states have wave vectors $\pm\pi/2$ and when $J_2=J_1=0$ they are particle-hole states with energy $2J_x$. As the interactions are switched on, the states descend (remaining degenerate by reflection symmetry) and, finally, at the (2,2) phase boundary they become degenerate with the two ground states of the BO phase. This is the basis for the numerical method of locating the phase boundary shown in Fig. 1.

Yet another view may be obtained by our starting from $J_x=0$. Group the spins in one of the (2,2) states into antiparallel pairs $[(+-)(-+)(+-)(-+)\cdots]$ and introduce a pseudospin τ^z_n which is $+1$ for $(+-)$ and -1 for $(-+)$. Then the state is antiferromagnetic in the τ^z_n and it has a partner obtained by the displacement of the (2,2) state by two sites or the τ_n variables by one site. This is a useful representation for small J_x because the J_x term in $\mathcal{H}$ can reverse a τ^z_n but not break a pair since it does not act on parallel spins. In this limit (small J_x), $\mathcal{H}$ reduces to an effective Hamiltonian

$$\mathcal{H}_{\text{eff}} = -\sum_n [2J_x\tau^x_n + (J_1 - 2J_2)\tau^z_n\tau^z_{n+1}], \tag{7}$$

which is an Ising model in a transverse field[18] and has a phase transition at $J_x = J_2 - J_1/2$ where the (2,2) order disappears. This line agrees well with the phase boundary obtained numerically.

A physical picture of our results may be given in the language of the one-dimensional electron gas: for $U \rightarrow \infty$ a $2k_F$ charge-density wave on the sites [(2,2) phase] always appears as a dimerization of a $4k_F$ charge-density wave on the bonds. The same qualitative picture should be valid for large but finite U. It will be of interest to study the model at finite temperatures to see how the various phases are first manifested as the temperature is reduced and to make a more direct connection with experiments on organic conductors.[5]

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