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Spin gap in a generalized one-dimensional t-J model

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The existence of a spin gap is studied in a generalization of the one-dimensional t-J model. A frustrated next-nearest-neighbor exchange interaction, J', gives rise to a spin gap at half-filling that survives for small doping and arbitrary values of J. Regions of phase separation and divergent superconducting fluctuations are distorted but still present in the extended model.

The phase diagram of the one-dimensional (1D) t-J model has been determined recently.[1,2] The supersymmetric model ($J=2t$) solved by Bethe-Ansatz techniques[3] is a Tomonaga-Luttinger (TL) liquid[4] for all values of the electron density.[5] Similar behavior is found for the entire region $0 \leq J/t \lesssim 1$ where the values of the correlation exponents are similar to those found in the one-band Hubbard model[6,7] in the region $U/4t \gtrsim 1$. Particularly, in the parameter region relevant for high-T_c superconductors ($n \sim 0.8$, $J/t \sim \frac{1}{3}$), the correlation exponents show dominant spin-density-wave correlations with suppression of superconducting correlations. Enhanced superconducting correlations were found only at values of $J/t \sim 3$ as a precursor of phase separation.[1] The high-T_c superconductors are, at least, two dimensional and while there are new types of instability possible in two dimensions such as d-wave superconductivity or flux phases, the experimental evidence points towards s-wave superconductivity. An s-wave state should have analogy in one dimension. This has motivated us to look for modifications of the t-J model that could show superconducting correlations at low doping.

A key test for s-wave superconductivity is the presence of a spin gap. In terms of weak-coupling theory known as "g-ology"[8] this occurs in the region with attractive backscattering matrix element ($g_1 < 0$) whereas a TL state occurs when $g_1 > 0$. In this paper we show that the addition to the t-J model of a frustrating next-nearest-neighbor exchange interaction, J', produces a spin gap for $n \lesssim 1$. A different model with an alternating exchange interaction was examined recently by Imada[9] but will not be considered here. In this context, it is worth remarking that recent neutron experiments by Rossat-Mignod and co-workers[10] show evidence for a spin gap opening up above T_c in the low doping compound $YBa_2Cu_3O_{6.69}$.

The t-J-J' model is written as

$$H = -t\sum_{i\sigma}(c_{i\sigma}^{\dagger}c_{i+1\sigma} + \text{H.c.}) + J\sum_{i}(\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \tfrac{1}{4} n_i n_{i+1}) + J'\sum_{i}(\mathbf{S}_i \cdot \mathbf{S}_{i+2} - \tfrac{1}{4} n_i n_{i+2}) . \quad (1)$$

Hereafter we set $t=1$. At half-filling, Majumdar and Ghosh[11] showed that a dimer state is the exact ground state at $J'/J = \frac{1}{2}$ and that the triplet excited state has an energy gap[12] equal to about $0.25J$. Continuum approximations[13] and the numerical study of small clusters[14] indicate that the gap opens for $J'/J > 0.25$. The properties of a single hole in a t-J-J' model were investigated by Doi *et al.*[15] The problem here is whether this spin gap survives when many holes are doped in this system. At first we will show the global feature of the phase diagram and then study several regions using analytical and approximate methods focusing on the spin gap. It is always difficult to confirm numerically the existence of a spin gap even in pure spin Hamiltonians as shown, for example, by the Haldane gap.[16,17] However, in this paper, we can show analytically the existence of a gap in the small-J limit by making use of the results for a spin chain.

Figure 1 shows the phase diagram for J'/J fixed at $\frac{1}{2}$. The detailed method for obtaining the boundary of the phase separation and the correlation exponent K_ρ is the

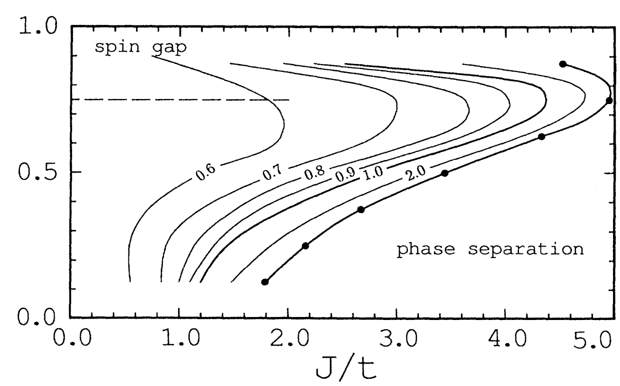

FIG. 1. Phase diagram of the one-dimensional t-J-J' model with $J'/J = 0.5$ determined from the 16-sites cluster calculation. The curves show the contours of constant correlation exponent K_ρ. They are calculated from a mesh of points similarly spaced in density in steps of $0.2J$. Solid symbols show the values where the inverse compressibility crosses zero representing the boundary of the phase separation.

same as that used for the t-J model.[1] The exponent K_ρ is determined from the relation[4,6,18] $K_\rho=\pi v_c n^2\kappa/\pi$, with v_c and κ being the charge velocity and the compressibility, respectively. The charge-density-wave (CDW) correlation decays as $e^{4ik_F r}/r^{4K_\rho}$ irrespective of the opening of a spin gap. However note that the other exponents are different in the two cases with and without a spin gap. Various exponents are summarized in Table I. It is apparent that the superconducting correlation becomes the most dominant when $K_\rho>1$ in both regions.

From Fig. 1, we can see that the boundary of the phase separation is more distorted compared to the 1D t-J model. Especially near $n=\frac{2}{3}$ it extends to the large-J regime. This is related to the fact that there is a stable configuration at this electron density, which we discuss below. Accompanying this distortion, the region with $K_\rho>1$ is also distorted, but remains adjacent to the phase separation as in the 1D t-J model. The low-density and high-density limit of the boundary can be understood easily. In the low-density limit, the two electron problem can be solved analytically. Two electrons form a singlet bound state at $J>4-2\sqrt{2}$ $(=1.172)$ for $J/J'=0.5$. This value is smaller than that in the t-J model ($J=2$) because the next-nearest exchange term also contributes to the attractive force between the electrons and shifts the boundary to smaller J. In the high-density limit, the boundary moves to a larger J.

Let us proceed to the problem of the opening of the spin gap. In the small-J limit, it can be shown that a wave function similar to the large-U limit of the 1D Hubbard model[7] is realized. At $J=0$ all the spin configurations are degenerate and thus the charge degrees of freedom of the wave function is expressed by the Slater determinant of spinless fermions, $(-1)^Q\det[\exp(ik_jx_{Ql})]$. Here $x_{Q1}<x_{Q2}<\cdots<x_{QN_e}$ are coordinates of all the electrons with Q being a permutation, and k_j are the momenta of free spinless fermions. In the perturbation procedure around this degenerate point,[7,19] the spin part of the wave function is determined by diagonalizing the following effective Hamiltonian for the squeezed spins:

$$H_{\rm eff}=(J\langle n_i n_{i+1}\rangle_{\rm SF}+J'\langle n_i(1-n_{i+1})n_{i+2}\rangle_{\rm SF})\sum_j \mathbf{S}_j\cdot\mathbf{S}_{j+1}$$
$$+J'\langle n_i n_{i+1} n_{i+2}\rangle_{\rm SF}\sum_j \mathbf{S}_j\cdot\mathbf{S}_{j+2}\,, \qquad (2)$$

where $\langle\cdots\rangle_{\rm SF}$ indicates the expectation value for spinless fermions. The summations over j are taken over the squeezed spin chain. This Hamiltonian is nothing but the J-J' Hamiltonian with effective exchange interactions, $J_{\rm eff}$ and $J'_{\rm eff}$. As a result, we see that the ground-state wave function in the small-J limit has a form, $(-1)^Q\times\det[\exp(ik_jx_{Ql})]\cdot\Phi(J'_{\rm eff}/J_{\rm eff})$, where Φ is the ground-state-spin wave function of (2). The ratio $J'_{\rm eff}/J_{\rm eff}$ is calculated simply from the expectation values and depends on the electron density. In the small doping regime, we find $J_{\rm eff}=(1-2\delta)J+\delta J'$ and $J'_{\rm eff}=(1-3\delta)J'$, where δ is the hole density, $\delta=1-n$. The effect of the doped holes is simply to reduce the effective exchange interactions so that the ratio decreases from the bare value $J'/J(=0.5$ in the present case). This means that the frustration of the spin chain is reduced by the doped holes, which is opposite to the intuitive expectation that doped holes induce frustration. The magnitude of the gap can be estimated from the results of the spin chain. Exact diagonalization of short spin-chains[14] showed that the gap decreases rapidly from $0.23J$ at $J'/J=0.5$ and becomes very small $(\sim 0.03J)$ at $J'/J=0.4$. Although it is difficult to determine precisely the critical value of J'/J at which the spin gap vanishes because it closes very slowly, it was estimated as approximately 0.25. Using the expectation values in the spinless fermions, we find that $J'_{\rm eff}/J_{\rm eff}$ becomes 0.4 already at $n=0.89$ and $J'_{\rm eff}/J_{\rm eff}=0.25$ at $n=0.75$. Figure 2 shows the obtained magnitude of the spin gap as a function of density. Note that the spin gap is easily destroyed by doping a few holes in the spin chain.

As we can expect from the J dependence of K_ρ near half-filling in Fig. 1, the J dependence of this spin gap region will be also small. To understand this behavior, we consider a variational wave function which is applied in the finite-J region. Assuming that the exchange term simply changes the spinless fermion part of the wave function, we use a variational state, $\chi(x_1,x_2,\ldots,x_{N_e};V)\Phi(J'_{\rm eff}/J_{\rm eff})$. χ is a ground-state wave function of a spinless fermion Hamiltonian with a nearest-neighbor attractive interaction V (t-V model). The ratio $J'_{\rm eff}/J_{\rm eff}$ is determined from the expectation values of $\langle n_i n_{i+1}\rangle_{\rm SF}$, etc., in the wave function χ. Using the exact solution of the XXZ Heisen-

TABLE I. Correlation exponents in the two cases without (TL liquid) and with a spin gap. SS and TS indicate singlet and triplet superconducting correlation, respectively.

Correlation	Without a spin gap	With a spin gap
$2k_F$ SDW	$1+K_\rho$	(exponential decay)
$2k_F$ CDW	$1+K_\rho$	K_ρ
SS	$1+1/K_\rho$	$1/K_\rho$
TS	$1+1/K_\rho$	(exponential decay)
$4k_F$ CDW	$4K_\rho$	$4K_\rho$

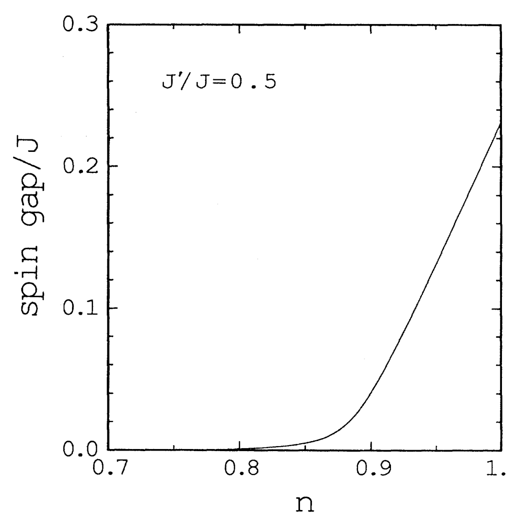

FIG. 2. Magnitude of spin gap as a function of electron density in the small-J limit. It is calculated from the exact ground-state wave function in this limit (see the text) combined with the numerical estimate of the spin gap at the half-filling (Ref. 14).

berg chain by Yang and Yang[20] which is equivalent to the t-V model, we can show that $\langle n_i n_{i+1}\rangle_{\rm SF} \sim 1-2\delta+4\pi^2\delta^4/3(2-V/t)^2$ near half filling. Obviously the effect of exchange term represented by V on the ratio $J'_{\rm eff}/J_{\rm eff}$ is very small. As a result, we expect that the spin gap region extends to fairly large-J values with the dependence on the electron density being roughly the same.

To investigate the possibility of a spin gap at large J, we study the special case with $n=\frac{2}{3}$. For the large-J region, a simple variational state is expected, which is an ordered state where one dimer and one hole alternate. This has an energy $-JN_e/2-J'N_e/8$. The actual ground state in the large-J limit is the completely phase separated state and it has an energy $-5JN_e/8-J'N_e/4$. We assume that the former state is realized just below the critical J for phase separation because it gains kinetic energy through a self-energy process in second-order perturbation theory. In the virtual state, one electron hops to its neighboring unoccupied site so that the state consists of one isolated electron and three electrons next to each other. By diagonalizing these four electrons in the virtual state, we can see that the excitation energy is $(J-J')/2$ and the matrix element is $\sqrt{3}/2$ for small J'. As a result, the energy gain from this second-order process is $-3t^2N_e/2(J-J')$. Comparing the above two variational states, we get the critical value of the phase separation at $J_c=4$ which is not far from the estimated value in Fig. 1 ($J_c \sim 4.5$).

As a direct estimate of the gap, we calculate the energies of the ground state ($S=0$) and the lowest $S=1$ state under periodic and antiperiodic boundary conditions in chains of increasing sizes:[21] $N_a=9$, 12, 15, and 18 at $n=\frac{2}{3}$. We fit to the formula

$$E_{S,\rm BC}(N_a)/N_a=\epsilon_\infty+S\Delta/N_a+C_{S,\rm BC}/N_a^2+SD_{\rm BC}/N_a^3+a_{S,\rm BC}\exp(-\xi/N_a)\;,$$

for $S=0,1$ where the coefficients depend on the total spin (S) and the boundary conditions (BC).[22] Minimizing the sum of least squares of the fit, we can see that the estimate of the spin gap, Δ, begins to increase in the range $4\le J\le 4.5$ just before phase separation at $J\sim 4.5$. The estimated value of Δ is very small ($\Delta<0.01t$). Although the spin gap could be a precursor to phase separation which we cannot resolve due to finite-size effects, we expect that the spin gap region at small J extends to $J=4$, $n=\frac{2}{3}$. Presumably the gap would be bigger at higher densities.

In this paper we have examined the doping of a frustrated spin chain with a spin gap. We show that the spin gap persists to finite values of the doping. This leads to a quantum liquid with enhanced CDW and singlet superconducting (SS) correlations. The relative strength of these correlations favors CDW for small values of J/t and SS for larger values of J/t. The magnitude of the spin gap reduces with hole doping, i.e., decreasing n. There is no evidence that doping induces frustration; rather, it reduces frustration and causes a transition to a TL liquid without a spin gap. In the high-T_c materials there is experimental evidence that there is a progression with increasing doping from antiferromagnetic long-range order to a quantum liquid with a spin gap above T_c to a quantum liquid which is close to a usual Fermi liquid. The one-dimensional model we discuss here shows behavior consistent with the latter type of crossover, i.e., from a frustrated quantum liquid with a spin gap to a TL liquid without a spin gap but does not show a crossover of the former type.

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[21] From the Bethe-Ansatz at $J=2$ and $J'=0$, we know that the odd number of sites does not affect the uniform convergence to the thermodynamic limit, contrary to what happens using odd number of electrons.

[22] We tried fitting to other formulas, for example without the exponential term. We found that the estimate of the spin gap changes only within $0.002t$, as we vary the fitting function.