Renormalization Group Analysis of the Spin-Gap Phase in the One-Dimensional t-J Model

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We study the spin-gap phase in the one-dimensional t-J model, assuming that it is caused by the backward scattering process. Based on the renormalization group analysis and symmetry, we can determine the transition point between the Tomonaga-Luttinger liquid and the spin-gap phases, by the level crossing of the singlet and the triplet excitations. In contrast to the previous works, the obtained spin-gap region is unexpectedly large. We also determine that the universality class of the transition belongs to the $k = 1$ SU(2) Wess-Zumino-Witten model. [S0031-9007(97)04331-7]

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The existence of a gap in the spin excitation has been considered to be a key to understanding high-T_c superconductivity. This stimulated the study of one-dimensional (1D) electron systems some years ago. Recently, possibilities of superconductivity in quasi-1D systems have been suggested [1], and understanding of spin-gap phase in (quasi-)1D systems increases the importance. Now, we reconsider this problem from the 1D t-J model which is the simplest, but not fully understood.

The Hamiltonian of the 1D t-J model is written as

$$\mathcal{H} = -t\sum_{i\sigma}(c_{i\sigma}^{\dagger}c_{i+1\sigma} + c_{i+1\sigma}^{\dagger}c_{i\sigma}) + J\sum_{i}(\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} - \hat{n}_i\hat{n}_{i+1}/4), \quad (1)$$

in the subspace without double occupancy. Generally, 1D electron systems belong to the universality class of Tomonaga-Luttinger (TL) liquid [2,3] which is characterized by gapless charge and spin excitations and power-law decay of correlation functions. The phase diagram of the 1D t-J model is obtained by Ogata *et al.*, using exact diagonalization [4]. They found the enhancement of the superconducting correlation ($K_c > 1$) and the phase separation ($K_c \to \infty$) for large J/t region. They also found a phase of singlet bound electron pairs in the very low density region, but could get no evidence for a spin-gap phase by using a finite size scaling method at $1/3$ filling. Hellberg and Mele studied this phase by using a Jastrow-type variational wave function [5]. In their approach, the variational parameter ν is related with K_c as $K_c = 1/(2\nu + 1)$. They found that there exists a finite region where the optimized parameter takes constant value $\nu = -1/2$ between the TL phase and phase-separated state, and they interpreted the region as the spin-gap phase. Another variational wave function is proposed by Chen and Lee [6].

However, these authors did not discuss the detailed mechanism of the spin-gap generation. One candidate of the spin-gap generation mechanism is due to the attractive backward scattering [scattering between electrons with the opposite momentum $(k_F, -k_F)$ and spin] [3,7]. In this case, the universality class of the transition is the $k = 1$ SU(2) Wess-Zumino-Witten (WZW) model [8]. On the basis of this assumption, we determine the transition point with the singlet-triplet level crossing method [8–10] and we obtain the phase diagram (Fig. 1). Then we will verify the consistency of our method, considering the ratio of the logarithmic correction term.

In general, the low-energy behavior of a 1D electron system is described by the U(1) Gaussian model (charge part) and the SU(2) sine-Gordon model (spin part) [3,11],

$$\mathcal{H} = \mathcal{H}_c + \mathcal{H}_s + \frac{2g_1}{(2\pi\alpha)^2}\int dx \cos\left(\sqrt{8}\phi_s\right). \quad (2)$$

Here α is a short-distance cutoff, g_1 is the backward scattering amplitude, and for $\nu = c, s$

$$\mathcal{H}_\nu = \frac{1}{2\pi}\int dx\left[v_\nu K_\nu(\pi\Pi_\nu)^2 + \frac{v_\nu}{K_\nu}\left(\frac{\partial\phi_\nu}{\partial x}\right)^2\right], \quad (3)$$

where Π_ν is the momentum density conjugate to ϕ_ν, $[\phi_\nu(x), \Pi_\nu(x')] = i\delta(x - x')$, K_ν is the Gaussian

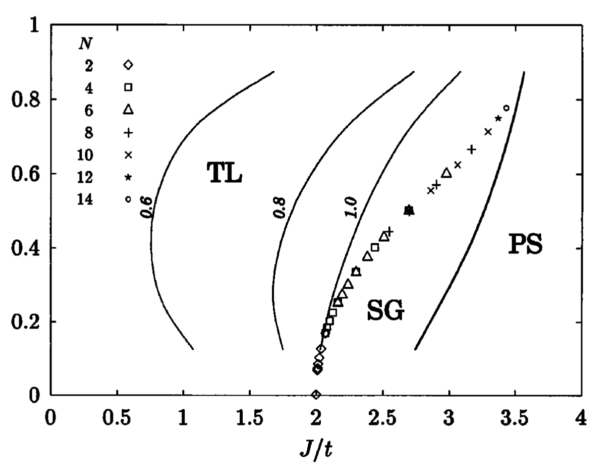

FIG. 1. Phase diagram of the 1D t-J model (TL: TL phase; SG: spin-gap phase; PS: phase-separated state). In the spin-gap phase where the backward scattering is attractive, the singlet excitation becomes lower than the triplet (see Figs. 2, 4). The contour lines of the K_c are calculated by the data of $L = 16$ system [31].

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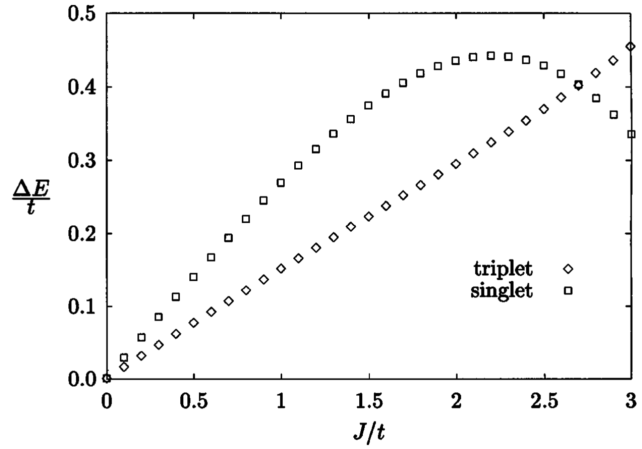

FIG. 2. Singlet and triplet excitation energies for $L = 16$ system at $n = 1/2$.

coupling, and v_c and v_s are charge and spin velocities, respectively. The primary field of this model is $\exp[i\sqrt{2}(m_\nu\phi_\nu + n_\nu\theta_\nu)]$, where the dual field is defined as $\partial_x\theta_\nu = \pi\Pi_\nu$. In TL phase ($g_1 > 0$), the parameters K_s and g_1 will be renormalized as $K_s^* = 1$ and $g_1^* = 0$, reflecting the SU(2) symmetry.

First, let us consider the case without renormalization, $g_1 = 0$. The finite size correction of the energy and the momentum of (3) are described by the conformal field theory (CFT) [12,13] with $c = 1$, where the central charge c characterizes the universality class of the model. For the t-J model, $c = 1$ as shown rigorously at $J/t = 2$ [17] and numerically [4]. The combined use of the CFT and the Bethe ansatz result gives a description of the 1D electron systems [14–17]. The ground state energy of the system under periodic boundary conditions is given by

$$E_0(L) = L\epsilon_0 - \frac{\pi(v_c + v_s)}{6L}c\,, \tag{4}$$

where L is the system size. The excitation energy and momentum are related with exponents as

$$E - E_0 = \frac{2\pi v_c}{L}x_c + \frac{2\pi v_s}{L}x_s\,, \tag{5}$$

$$P - P_0 = \frac{2\pi}{L}(s_c + s_s) + 4k_F D_c + 2k_F D_s\,, \tag{6}$$

where $k_F = \pi N/2L$ with electron number N, and the scaling dimensions and the conformal spins are defined by $x_\nu = \Delta_\nu^+ + \Delta_\nu^-, s_\nu = \Delta_\nu^+ - \Delta_\nu^-$, respectively, with the conformal weights

$$\Delta_\nu^\pm = \frac{1}{2}\left(\sqrt{\frac{K_\nu}{2}}\,m_\nu \pm \frac{n_\nu}{\sqrt{2K_\nu}}\right)^2 + N_\nu^\pm\,. \tag{7}$$

The variables m_ν and n_ν are related with electron quantum numbers as $m_c = 2D_c + D_s, n_c = \Delta N_c/2, m_s = D_s, n_s = \Delta N_s - \Delta N_c/2$. Here ΔN_c is the change of the total number of electrons, and ΔN_s is the change of the number of down spins. D_c (D_s) denotes the number of particles moved from the left charge (spin) Fermi point to the right one. $N_c^\pm$ ($N_s^\pm$) is characterized by simple particle-hole excitations near right or left charge (spin) Fermi points.

These quantum numbers are restricted by the selection rule under periodic boundary conditions [14]

$$D_c = \frac{\Delta N_c + \Delta N_s}{2} \qquad (\mathrm{mod}\ 1)\,, \tag{8a}$$

$$D_s = \frac{\Delta N_c}{2} \qquad (\mathrm{mod}\ 1)\,. \tag{8b}$$

In the case of twisted boundary conditions $c_{j+L,\sigma}^\dagger = e^{i\Phi}c_{j\sigma}^\dagger$ which is equivalent to the system where the flux Φ penetrates the ring [18], D_c is modified as $D_c + \Phi/2\pi$. For the ground state E_0, we choose periodic boundary conditions ($\Phi = 0$) for $N = 4m + 2$ electrons and antiperiodic boundary conditions ($\Phi = \pi$) for $N = 4m$ electrons with an integer m. Changing the boundary conditions, the ground state becomes always singlet with zero momentum ($P_0 = 0$) [4,19].

In order to eliminate the contribution of the charge part, and extract the singlet and the triplet excitation in the spin part ($x_s = 1/2$), we turn our attention to the following states: $(\Delta N_c, \Delta N_s, D_c, D_s) = (0, \pm 1, 0, 0), (0, 0, \mp 1/2, \pm 1)$ under twisted boundary conditions ($\Phi = \pi$ for $N = 4m + 2$, $\Phi = 0$ for $N = 4m$). We can identify these excitation spectra by using (5) and (6), but the momentum P and the wave number p are not always identical. There is a relation $P = p - \Phi N/L$ between them [20].

Next, we consider the renormalization ($g_1 \neq 0$). By the change of the cutoff $\alpha \to e^{dl}\alpha$, the coupling constant g_1 and K_s are renormalized as [21]

$$\frac{dy_0(l)}{dl} = -y_1^2(l)\,, \tag{9a}$$

$$\frac{dy_1(l)}{dl} = -y_0(l)y_1(l)\,, \tag{9b}$$

where $y_1(l) = g_1/\pi v_s, K_s = 1 + y_0(l)/2$. For the SU(2) symmetric case $y_0(l) = y_1(l)$, and $y_0(l) > 0$, the scaling dimensions of the operators for singlet and triplet excitations $\sqrt{2}\cos\sqrt{2}\phi_s$ (x_{ss}), and $\sqrt{2}\sin\sqrt{2}\phi_s$, $\exp(\mp i\sqrt{2}\theta_s)$ (x_{st}) split logarithmically by the marginally irrelevant coupling as [22]

$$x_{ss} = \frac{1}{2} + \frac{3}{4}\frac{y_0}{y_0\ln L + 1}\,, \tag{10a}$$

$$x_{st} = \frac{1}{2} - \frac{1}{4}\frac{y_0}{y_0\ln L + 1}\,, \tag{10b}$$

where y_0 is the bare coupling, and we have set $l = \ln L$. This result is equivalent to that of the $k = 1$ SU(2) WZW model [8]. Note that the ratio of the logarithmic corrections are given by Clebsch-Gordan coefficients.

When $y_0 < 0$, $y_0(l)$ is renormalized to $y_0(l) \to -\infty$, and there appears a spin gap. At the critical point ($y_0 = 0$), there are no logarithmic corrections in the excitation gaps. The physical meaning of this point is that the backward scattering coupling changes from repulsive to attractive. And the SU(2) symmetry is enhanced at the critical point to the chiral SU(2) $\times$ SU(2) symmetry [8], since the spin degrees of freedom of the right and the left Fermi points become independent. Therefore, the critical point is obtained from the intersection of the singlet and the triplet excitation spectra [8–10]. Using this method, we can determine the critical point with high precision [10], since the remaining correction is only $x_s = 4$ irrelevant fields [23,24].

Here we analyze the numerical results for the t-J model (1) with the above explained method. We diagonalize $L = 8-30$ systems by the use of the Lanczos and Householder method. An example of data ($L = 16, n \equiv N/L = 1/2$) is shown in Fig. 2. Since the critical point is almost independent of the system size as is shown in Fig. 3, the phase diagram can be constructed without extrapolation. Our result is similar to Hellberg and Mele's in the low density region, but the spin-gap phase spreads extensively toward the high density region. We are not able to answer whether the spin gap survives in the $n \to 1$ limit or not, because the numerical results become unstable in the high density region where the phase boundary is close to the phase-separated state. In TL phase, singlet and triplet superconducting correlations (SS, TS) have the same critical exponent $1/K_c + 1$ [3], while with a spin gap, TS decays exponentially and SS is enhanced as $1/K_c$, so that SS is dominant in the spin-gap region.

In order to check the consistency of our argument, we calculate the ratios of the logarithmic corrections and scaling dimensions for the singlet and the triplet excitations from (5) and (10). Here the spin wave velocity is given by [25]

$$v_s = \lim_{L\to\infty} \frac{E(L,N,S=1,P=2\pi/L) - E_0(L,N)}{2\pi/L}, \tag{11}$$

which is extrapolated by the function $v_s(L) = v_s(\infty) + A/L^2 + B/L^4$. These corrections are explained by the irrelevant fields. The average of the renormalized scaling dimension $(x_{ss} + 3x_{st})/4$, eliminating logarithmic corrections, and its finite size effect are shown in Fig. 4 and Fig. 5, respectively. The extrapolated data become $1/2$ with error less than 0.2%.

Finally, we discuss the reason why the previous studies have estimated the spin-gap region to be very much narrower than the real one. From the two-loop renormalization group equation of the $k = 1$ SU(2) WZW model [26–28]

$$\frac{dy_0(l)}{dl} = -y_0^2(l) - \frac{1}{2}y_0^3(l), \tag{12}$$

the spin gap ΔE grows singularly as

$$\Delta E \propto \sqrt{J - J_c}\exp[-\mathrm{const}/(J - J_c)], \tag{13}$$

where $y_0 \propto J_c - J$, therefore it is very difficult to find the critical point using the conventional finite size scaling method. Note that (13) is the same asymptotic behavior as the spin gap of the negative U Hubbard model at half-filling, which can be obtained from the charge gap at positive U [29], and the transformation between the charge and the spin degrees of freedoms [30].

In conclusion, we studied the spin-gap phase in the 1D t-J model, considering the backward scattering effect in the TL liquid by the renormalization group analysis. Using the twisted boundary conditions, we can extract the spin excitation spectra and determine the critical point as

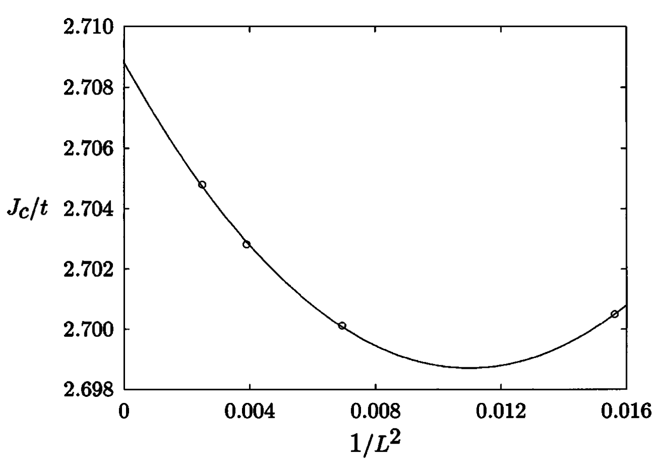

FIG. 3. Size dependence of J_c/t determined by the intersections of the excitation spectra for $L = 8, 12, 16, 20$ systems at $n = 1/2$. These points are fitted by the form $A + B/L^2 + C/L^4$.

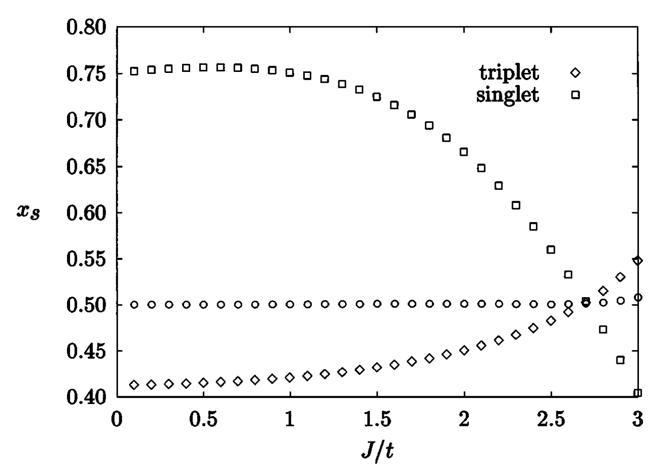

FIG. 4. Extrapolated value of $(x_{ss} + 3x_{st})/4$ and the scaling dimensions for the singlet (x_{ss}) and the triplet (x_{st}) excitations for $L = 16$ system at $n = 1/2$.

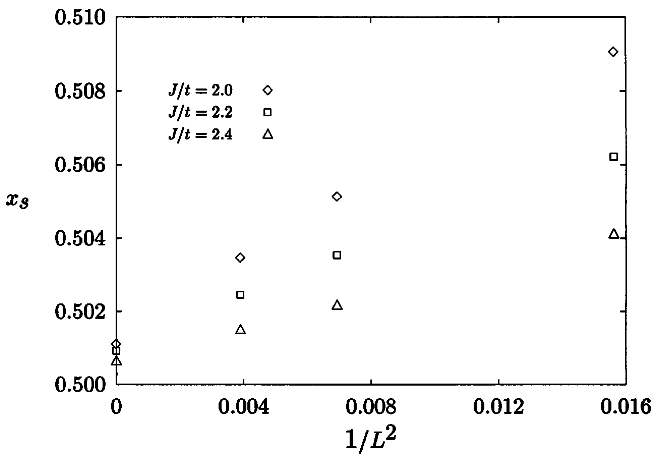

FIG. 5. Size dependence of the averaged scaling dimension $(x_{ss} + 3x_{st})/4$ at $n = 1/2$.

in spin systems. The phase boundary is determined by the point where the backward scattering becomes repulsive to attractive. The spin-gap phase obtained in this way is unexpectedly large, and the consistency of the argument is also checked. This method can be applied to other models in 1D electron systems, if the SU(2) symmetry is assured.

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[1] E. Dagotto and T. M. Rice, Science **271**, 618 (1996).
[2] F. D. M. Haldane, J. Phys. C **14**, 2585 (1981).
[3] J. Sólyom, Adv. Phys. **28**, 201 (1979).
[4] M. Ogata, M. U. Luchini, S. Sorella, and F. F. Asaad, Phys. Rev. Lett. **66**, 2388 (1991).
[5] C. S. Hellberg and E. J. Mele, Phys. Rev. B **48**, 646 (1993).
[6] Y. C. Chen and T. K. Lee, Phys. Rev. B **47**, 11 548 (1993).
[7] N. Manyhárd and J. Sólyom, J. Low Temp. Phys. **12**, 529 (1973).
[8] I. Affleck, D. Gepner, H. J. Schulz, and T. Ziman, J. Phys. A **22**, 511 (1989).
[9] T. Ziman and H. J. Schulz, Phys. Rev. Lett. **59**, 140 (1987).
[10] K. Okamoto and K. Nomura, Phys. Lett. A **169**, 433 (1992); K. Nomura and K. Okamoto, J. Phys. A **27**, 5773 (1994).
[11] H. J. Schulz, Phys. Rev. Lett. **64**, 2831 (1990); Int. J. Mod. Phys. B **5**, 57 (1991).
[12] H. W. J. Blöte, J. L. Cardy, and M. P. Nightingale, Phys. Rev. Lett. **56**, 742 (1986); I. Affleck, Phys. Rev. Lett. **56**, 746 (1986).
[13] J. L. Cardy, J. Phys. A **17**, L385 (1984).
[14] F. Woynarovich, J. Phys. A **22**, 4243 (1989).
[15] H. Frahm and V. E. Korepin, Phys. Rev. B **42**, 10 553 (1990).
[16] P. -A. Bares and G. Blatter, Phys. Rev. Lett. **64**, 2567 (1990); P.-A. Bares, G. Blatter, and M. Ogata, Phys. Rev. B **44**, 130 (1991).
[17] N. Kawakami and S. K. Yang, Phys. Rev. Lett. **65**, 2309 (1990); J. Phys. Condens. Matter **3**, 5983 (1991).
[18] W. Kohn, Phys. Rev. **133**, A171 (1964); B. S. Shastry and B. Sutherland, Phys. Rev. Lett. **65**, 243 (1990).
[19] M. Ogata and H. Shiba, Phys. Rev. B **41**, 2326 (1990).
[20] The unitary operator $\exp(-i\Phi \sum_{j=1}^{L} j\hat{n}_j/L)$ transforms the wave number defined in the translationally invariant system as $p - \Phi N/L$ in the system with the twisted boundary conditions.
[21] J. M. Kosterlitz, J. Phys. C **7**, 1046 (1974).
[22] T. Giamarchi and H. J. Schulz, Phys. Rev. B **39**, 4620 (1989).
[23] J. L. Cardy, Nucl. Phys. B **270**, 186 (1986).
[24] P. Reinicke, J. Phys. A **20**, 5325 (1987).
[25] The quantum numbers corresponding to the excitation for the spin velocity are $(\Delta N_c, |\Delta N_s|, D_c, D_s) = (0, 1, \pm 1/2, \mp 1)$ or $(N_s^+, N_s^-) = (1, 0), (0, 1)$. All these states have momentum $P = \pm 2\pi/L$, and form the SU(2) triplets.
[26] D. J. Amit, Y. Y. Goldschmidt, and G. Grinstein, J. Phys. A **13**, 585 (1980).
[27] C. Destri, Phys. Lett. B **210**, 173 (1988); **213**, 565E (1988).
[28] K. Nomura, Phys. Rev. B **48**, 16 814 (1993).
[29] A. A. Ovchinikov, Zh. Eksp. Teor. Fiz. **57**, 2137 (1969) [Sov. Phys. JETP **30**, 1160 (1970)].
[30] H. Shiba, Prog. Theor. Phys. **48**, 2171 (1972).
[31] The contour lines of K_c shift larger J/t side in the high density region comparing with the result obtained by Ogata *et al.* We determined K_c by using the relation $K_c = \pi\sqrt{Dn^2\kappa/2}$ where D is the Drude weight and κ is the compressibility. This way of calculation has less size dependence near the phase separation {see M. Nakamura and K. Nomura, cond-mat/9702126) [Phys. Rev. B (to be published)]}.