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Critical line of the $SU(2)$ spin-gap transition in the one-dimensional t–U–J model

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Abstract

We investigate the phase diagram of the half-filled one-dimensional t–U–J model by the level-spectroscopy method. Due to the competition between the Coulomb repulsion U and the antiferromagnetic exchange J, the backward scattering may change sign from repulsive to attractive, leading to spin-gap instability. From the excitation spectra of finite-size clusters, the transition line $U_c(J)$ can be accurately determined in the weak-coupling and intermediate-coupling regimes. With increasing J, $U_c(J)$ deviates from that given by the weak-coupling theory based on the spin–charge separation hypothesis. Moreover, we find that the spin gap vanishes robustly when $U \gtrsim 0.35t$, irrespective of J.

The quantum states of an electron liquid with unbroken spin-rotational symmetry are of particular interest in strongly correlated electron systems, especially in high-temperature cuprate superconductors. Anderson [1] first proposed the idea of the resonating valence bond (RVB) state as such a characteristic spin liquid for the correlated electrons in the 2D Cu–O plane. Recently, Laughlin [2] suggested that a gossamer superconducting state can arise from an antiferromagnetic Mott insulator if double occupation is allowed. Zhang [3] showed further that the gossamer superconducting state can evolve smoothly into the RVB spin-liquid phase in a 2D t–U–J model. It is remarkable that, as the basic feature of doped RVB states, the spin–charge separation is well established only in 1D systems so far, and the superconductivity may take place if the spin excitations have an energy gap. It is widely accepted that in 1D a symmetry preserving gapped spin-liquid phase is possible in Haldane spin chains [4], while in other cases its appearance needs spin rotational symmetry breaking, translational symmetry breaking (or explicit dimerizations), inter-chain couplings, or other kinds of explicit frustration. For 1D itinerant electron systems, though Oshikawa showed that a finite excitation gap is possible if the particle number per unit cell is an integer [5], few 1D systems composed of a pure single chain which respect all the desired symmetries and without explicit frustrations are known to exhibit gapped spin-liquid states at half-filling.

Recently, based mainly on analytical bosonization and numerical transfer matrix-renormalization group methods, it has been found that such a spin-liquid phase is indeed realized in a half-filled itinerant electron system described by the one-dimensional t–U–J model [6].

$$H = -t\sum_{i\sigma}\left(c^{\dagger}_{i\sigma}c_{i+1\,\sigma} + \text{h.c.}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + J\sum_{i}\mathbf{S}_i\cdot\mathbf{S}_{i+1}. \tag{1}$$

When J is anisotropic, i.e., spin-rotational $SU(2)$ symmetry is broken to $U(1)$, the corresponding model was studied by Japaridze *et al* in the large-bandwidth limit [7]. They predicted a transition to the dimerized ordering phase in the case of weak anisotropy by assuming spin–charge separation in the weak-coupling regime. However, except in the weak-coupling regime and a special point $J \sim t$ in the intermediate-coupling regime [6], the existence of a gapped spin-liquid phase (with spontaneous dimerization) in the isotropic antiferromagnetic case in the intermediate- and strong-coupling regimes has not been clarified. Notice that a similar spin-liquid state, characterized by the bond-charge-density wave (BCDW) or spontaneous dimerization, was discovered in the conventional extended Hubbard model (EHM) with the nearest-neighbour Coulomb repulsion [8–10] or in the ionic Hubbard model with alternative potential [11], where its existence is due to the interplay of the bond insulator characterized by the charge-density wave (CDW) and the Mott insulator characterized by the spin-density wave (SDW). The two competing insulating phases exist even in the atomic limit. However, the gapped spin-liquid phase in the t–U–J model is quite unusual. One expects that it develops in the intermediate regime and vanishes at either free or atomic limits inside the Mott insulator [6]. It is interesting to clarify the generic feature of the boundary line between the spin-gapless (SDW) and gapped (BCDW) states in the Mott insulating phase of this model.

In this paper, we shall show further numerical evidence for the existence of the gapped spin-liquid phase and determine the generic phase diagram of the t–U–J model by the level-spectroscopy method. It is known that though the spin-gap transition can be analysed by the weak-coupling theory based on the bosonization and renormalization group (RG), its validity is ensured only in the weak-coupling limit [12–15]. On the other hand, direct numerical calculation of the gap based on the conventional finite-size scaling method is very difficult, since the gap opens very slowly near the critical point. Instead of direct evaluation of the gap, the level-spectroscopy method investigates the ground-state phase diagram by using the excitation spectra of finite-size clusters [8, 16, 17]. By taking into account the logarithmic corrections to the Tomonaga–Luttinger liquid (TLL) from the backward scattering, its validity is ensured in both the weak- and intermediate-coupling regimes. This method was initiated by Julien and Haldane [16] and extensively developed by Nomura and Okamoto [17] in the study of the $S = 1/2$ frustrated spin chains, and has been also successfully applied to 1D electron systems by Nakamura *et al* [8, 18]. Here, by using this method, we investigate the phase diagram of the t–U–J model from the data of the excitation spectra of finite-size clusters. The obtained transition line $U_c(J)$ is in good agreement in the weak-coupling regime with the weak-coupling theory. With increasing J in the intermediate-coupling regimes, $U_c(J)$ deviates from the weak-coupling prediction, showing the significant spin–charge coupling effects. Moreover, we find that the spin gap vanishes robustly when $U \gtrsim 0.35t$ irrespective of J.

Let us first briefly describe the spin-gap scenario in the weak-coupling theory based on the bosonization and RG [12–15]. The electron operator $c_{j,\sigma}$ is described by continuous fermion fields expanded at the two Fermi points

$$c_{j,\sigma} \approx \psi_{\mathrm{L},\sigma}(x)\mathrm{e}^{-\mathrm{i}k_{\mathrm{F}}x} + \psi_{\mathrm{R},\sigma}(x)\mathrm{e}^{\mathrm{i}k_{\mathrm{F}}x}. \tag{2}$$

The low-energy excitations are then described by the charge and spin bosonic fields through the $U(1)$ representation

$$\psi_{r,\sigma} = \frac{1}{\sqrt{2\pi a}} \mathrm{e}^{\mathrm{i}\sqrt{\pi/2}[r(\phi_c+\sigma\phi_s)-(\theta_c+\sigma\theta_s)]} \tag{3}$$

where a is a short-distance cut-off (lattice constant) and r and σ in the rhs refer to $+/-$ for right/left and up/down fields respectively. The field ϕ_ν and the dual field θ_ν of the charge ($\nu = c$) and spin ($\nu = s$) sectors satisfy the relation $[\phi_\nu(x), \theta_{\nu'}(x')] = -\mathrm{i}\pi\delta_{\nu\nu'}\mathrm{sgn}(x - x')/2$. Then the effective low-energy Hamiltonian density is given by

$$H = H_c + H_s + H_{cs}, \tag{4}$$

$$H_\nu = \frac{v_\nu}{2\pi}[K_\nu(\partial_x\theta_\nu)^2 + K_\nu^{-1}(\partial_x\phi_\nu)^2] + \frac{g_\nu}{2\pi^2 a}\cos\sqrt{8\pi}\phi_\nu, \tag{5}$$

$$H_{cs} = -\frac{g_{cs}}{2\pi^2 a}\cos\sqrt{8\pi}\phi_c\cos\sqrt{8\pi}\phi_s. \tag{6}$$

The parameters K_ν and v_ν are the Gaussian coupling and the velocity of the elementary excitations, respectively. The other three couplings describe the non-TLL-type processes: the umklapp scattering ($g_c = -g_{3\perp}$), the backward scattering ($g_s = g_{1\perp}$), and the spin–charge coupling ($g_{cs} = g_{3\|}$). Notice that for the charge sector $K_c = [1 + (U + 3J/2)/\pi t]^{-1/2} < 1$ while for the spin sector K_s is renormalized as $K_s = 1$, keeping the $SU(2)$-spin rotational symmetry.

According to the RG argument, the energy scale of H_{cs} is large than those of others, this term can be neglected in the weak-coupling regime so that spin–charge separation occurs. For the charge sector, the RG equation predicts that the Gaussian fixed line $g_c = 0$ is stable for $g_c \geqslant 0$, but unstable for $g_c < 0$. Because the initial value is given by $g_c = U + 3J/2 > 0$ in the t–U–J model, so the charge gap opens. Similarly, for the spin sector, the RG equation predicts a spin gap when the initial $g_s = U - J/2 < 0$. So in the weak-coupling regime of the half-filled t–U–J model, there is a finite gap in charge excitations for all positive U and J, while there is a finite gap in spin excitations for $J > U/2$. However, with increasing J from the weak- to intermediate-coupling regime, the spin–charge coupling becomes less irrelevant, so that H_{cs} cannot be neglected. By taking into account this coupling, the corresponding RG equations have been solved and it has been found that the phase boundary deviates significantly below the line $J = U/2$ [6].

Of course, the above RG description on the phase transition is restricted in the weak-coupling regime, though it is also often expected to be applicable qualitatively in part of the intermediate regime. To determine the phase transition boundary in a wider regime quantitatively, we use the Lanczos algorithm to diagonalize finite-size clusters and analysis the data by the level-spectroscopy method. Based on the TLL theory (equivalent to $c = 1$ conformal field theory), the level-spectroscopy method considers the renormalization of the Umklapp and backward scatterings as well as their logarithmic corrections [8].

In the absence of the non-linear terms ($g_c = g_s = g_{cs} = 0$), the system is exactly solvable; the excitation spectra are determined by quantum numbers n_ν and m_ν, respectively, where n_ν denotes excitations involving the variation of particle numbers in sector ν (=c, s) and m_ν denotes the corresponding current excitations (from left Fermi to right Fermi points). For a given excitation in the ν-sector, define the scaling dimension $x_\nu = \frac{1}{2}(\frac{{n_\nu}^2}{K_\nu} + m_\nu^2 K_\nu)$ and the conformal spin $s_\nu = n_\nu m_\nu$ respectively; the excitation spectra and their wavenumbers are then given by

$$\Delta E = \frac{2\pi v_c}{L}x_c + \frac{2\pi v_s}{L}x_s, \tag{7}$$

$$k = \frac{2\pi}{L}(s_c + s_s) + 2m_c k_{\mathrm{F}} \tag{8}$$

with L and $k_{\mathrm{F}} = \pi N/2L$ being the length of the system and the Fermi wavenumber respectively.

Now assume that the excitations move adiabatically when the non-linear terms are added to the system. The conformal field theory [19, 20] says that there is a (perturbation) operator $\mathcal{O}(r)$ with scaling dimensions x_ν which changes the ground-state energy to the excited one with the same scaling dimensions, i.e., there is one to one correspondence between the excitation spectra and the operator:

$$\langle \mathcal{O}(r)\mathcal{O}(r')\rangle \sim \mid r - r' \mid^{-2(x_c+x_s)} . \tag{9}$$

The operators corresponding to the excited states are given by

$$\mathcal{O}_{n_\nu, m_\nu} \propto \mathrm{e}^{\mathrm{i}\sqrt{2}(n_\nu\theta_\nu + m_\nu\phi_\nu)}. \tag{10}$$

In our analysis we shall focus on the excitation spectra which correspond to the following operators:

$$\mathcal{O}_1 \equiv \sqrt{2}\cos\sqrt{2}\phi_s \tag{11}$$

$$\mathcal{O}_2 \equiv \sqrt{2}\sin\sqrt{2}\phi_s \tag{12}$$

$$\mathcal{O}_3 \equiv \sqrt{2}\mathrm{e}^{\pm\mathrm{i}\sqrt{2}\phi_s} \tag{13}$$

relating the singlet ($\mathcal{O}_1$) and triplet ($\mathcal{O}_2$, $\mathcal{O}_3$) states. Upon spin–charge separation, their scaling dimensions in the gapless phase are 1/2 for the infinite system, but split each other logarithmically for a finite-size system as follows:

$$x_{\sigma 1} = \frac{1}{2} + \frac{3}{4}\frac{y}{y\ln L + 1} \tag{14}$$

$$x_{\sigma 2} = x_{\sigma 3} = \frac{1}{2} - \frac{1}{4}\frac{y}{y\ln L + 1} \tag{15}$$

with $y = g_s/\pi v_s$. At the critical point (the fixed point $y = 0$) there are no logarithmic correction in the excitation gap. Therefore, the level crossing of $\Delta E_{\sigma,1}$ and $\Delta E_{\sigma,3}$ excitations serves as a good estimator for the spin-gap transition, even in the case when the scaling dimensions deviate from equations (14) and (15) with increasing spin–charge couplings.

To numerically identify the excitation spectra, the discrete symmetries of the wavefunctions for the excited states are useful and are specified by those of the ground state and the operators. The discrete symmetry operations are particle–hole ($\mathcal{C}$), $c_{j\sigma} \leftrightarrow (-1)^j c^\dagger_{j\sigma}$; space inversion ($\mathcal{P}$), $c_{j\sigma} \leftrightarrow c_{L-j+1\sigma}$; and spin reversal ($\mathcal{T}$), $c_{j\sigma} \leftrightarrow c_{j-\sigma}$; see table 1 in [8]. Here, $\mathcal{P} = \mathcal{T} = 1$ for the singlet state and $\mathcal{P} = \mathcal{T} = -1$ for the triplet state. We diagonalize the systems with $L = 10, 12$, and 14, where the Lanczos algorithm was used to obtain eigenvalues of the Hamiltonian in the corresponding subspaces. At half-filling, the (anti-) periodic boundary condition is used for system size $L/2 =$ (even) odd to obtain a singlet ground state. The spin-gap transition lines obtained are shown in figure 1.

In figure 1, we see that our numerical results in the weak-coupling limit show that the boundary line is given by $U_{\mathrm{c}} = J/2$, which is accurately predicted by bosonization and RG arguments assuming the spin–charge separation. With increasing interaction J, the boundary line considerably deviates from this behaviour. But in part of the intermediate regime, where $J \simeq 0.2t \sim 1.0t$, the deviation can be also predicted qualitatively by the RG argument provided the spin–charge coupling term is taken into account [6]. This means that the level-spectroscopy method enables us to access the elementary excitations described by the effective field theory at least in the regime of $J = 0 \sim 1.0t$. In fact, the phase boundary determined by the level-spectroscopy method is reliable in the weak- and intermediate-coupling regimes (for it takes into account the logarithmic corrections); it is not guaranteed in the strong-coupling

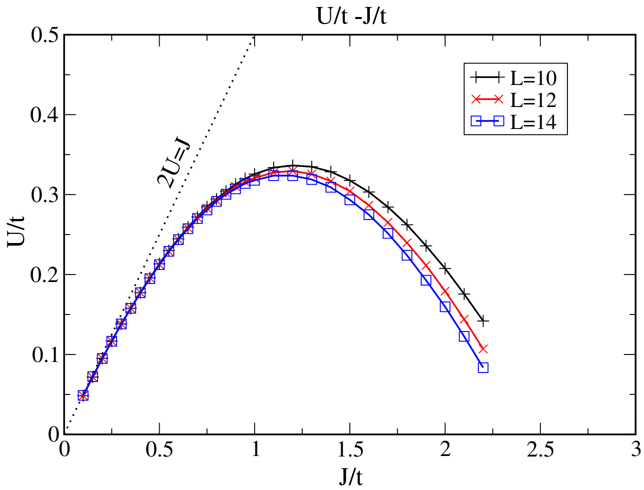

Figure 1. The $SU(2)$ spin-gap transition line of the one-dimensional t–U–J model obtained by the level-spectroscopy method in the finite systems with $L = 10, 12, 14$. The dotted line $2U = J$ is the critical line predicted by the weak-coupling theory based on the spin–charge separation hypothesis. (This figure is in colour only in the electronic version)

regime. We see that the finite-size effects become significant when $J \gtrsim 2t$. So the results shown in figure 1 in the strong-coupling regime may not necessary indicate a finite fixed point J_c. Instead, we believe that the fixed point J_c (the spin gap vanishes when $J > J_c$), if it exists, should be ∞. This can be understood by examining the instability of the spin gap against the backward scattering in the limit when $t \to 0$ and $J \gg U$. In this limit, the excitations of the charge field are strongly suppressed so that ϕ_c is pinned at its vacuum expectation, and the corresponding $K'_c = (\frac{t}{t+(U+3J/2)\pi})^{1/2} \to 0$ as $t \to 0$. We may bosonize the Heisenberg chain and treat the kinetic and Coulomb energies as perturbations. (The prime is used to distinguish the parameters from those appearing in the weak-coupling regime.) The effective Hamiltonian density is obtained as

$$H_{\text{eff}} = \frac{v'_s}{2\pi}[(\partial_x\phi_s)^2 + (\partial_x\theta_s)^2] + \frac{g'_s}{2\pi^2 a}\cos\sqrt{8\pi}\phi_s \tag{16}$$

with $v'_s \approx 3J$. Here we neglect the charge excitations as they are all strongly suppressed; their feedback on the spin excitations is encoded in $g'_s = U - \frac{1}{2}(1-\lambda)J$, where $\lambda \equiv \langle\cos 2\sqrt{2\pi}\phi_c\rangle$ is the vacuum expectation value of the charge coupling. It can be approximated by $\simeq (g'_c/v'_c)^{K'_c/(1-K'_c)} \approx 1^-$ as $K'_c \to 0$. Thus the backward scattering is irrelevant for $g'_s > 0$ and relevant for $g'_s < 0$; the latter case indicates the spin-gap instability. The line of $g'_s = 0$ is given by $2U = (1-\lambda)J$. Because $\lambda \to 1^-$ much faster than the increase of J, $(1-\lambda)J \to 0^+$ when $t/J \to 0$. Therefore, the spin-gap phase persists but is strongly suppressed for sufficiently large J.

As an important byproduct of our numerical calculations, we see that there exists a critical point $U_c \approx 0.35t$ while for $U > U_c$ the spin gap vanishes, irrespective of J. Notice that the crossing point where U_c takes the maximal value $0.35t$ is about $J \simeq 1.25t$. This numerical result is reliable, as it just locates in the regime where the finite-size effect is not significant and the level-spectroscopy method is guaranteed. Anyway, its precise location should not be far away from this point, because the phase boundary must approach the J-axis at either limit. The existence of small U_c is quite interesting and is beyond the prediction of the conventional weak-coupling theory. It means that in the BCDW phase of a Mott insulator the spin gap driven by the double occupation and the interplay between kinetic energy and antiferromagnetic exchange can be significantly suppressed by a fairly small on-site Coulomb repulsion.

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