Phase Diagram of the One-Dimensional t-J Model

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The phase diagram of the one-dimensional t-J model is investigated by analyzing the results of exact diagonalization and the exact solutions at $J/t=0$ and 2. Phase separation takes place above a critical value of J around $J_c/t=2.5$–3.5 depending on the electron density. In the small-J region, Tomonaga-Luttinger liquid theory holds and its correlation exponents are calculated as a function of J/t and the electron density. Superconducting correlations become dominant in a region between the solvable case ($J/t=2$) and phase separation. A spin-gap region is also found at low density.

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The t-J model is one of the simplest models for studying strongly correlated electron systems and is a most important problem for high-T_c superconductivity. Although high-T_c cuprates are at least two-dimensional (2D) systems, it is also interesting to investigate the one-dimensional (1D) model. It is relatively easy to explore and, as Anderson recently claimed,[1] 2D strongly correlated systems could share some properties of the 1D case.

Interacting 1D electron systems generally behave as Tomonaga-Luttinger (TL) liquids[2,3] in which the correlation functions have power-law decays with exponents which depend on the interaction strength. For systems with spin rotational invariance, all the exponents depend only on one parameter. Therefore the phase diagram for these 1D models is determined by the calculation of one correlation exponent as a function of electron density n and the magnitude of the interaction.

For the 1D Hubbard model, the exact solution was explicitly obtained a long time ago for every value of n and U/t.[4] However, only very recently have the exponents in the whole phase diagram been calculated,[5-10] using a simple relation between them and the spectrum of the low-lying states. On the other hand, the 1D t-J model

$$H=-t\sum_{(i,j)\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+J\sum_{(i,j)}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}n_in_j), \quad (1)$$

defined on the subspace without double occupancy, is exactly solvable only at $J/t=2$ in this notation,[11-13] where (i,j) means the summation over nearest-neighbor pairs. Therefore it is more difficult to obtain its phase diagram. The purpose of this paper is to calculate it by using the results of exact diagonalization, the exact solutions, and various well-known results for different limiting cases. Hereafter we set $t=1$.

In the limit of $J\to 0$, the t-J model is equivalent to the $U/t\to\infty$ Hubbard model, because first-order perturbation theory[5] around $J=0$ and $U/t=\infty$ gives the same ground-state wave function in both cases. The $U/t\to\infty$ Hubbard model has rigorously been shown to behave as a TL liquid.[8-10] Quite recently it has been shown that the solvable case ($J=2$) is also a TL liquid and the behavior of the correlation exponent has been obtained.[14] Therefore, unless some instability occurs, the t-J model behaves as a TL liquid. We will identify two such instabilities: phase separation and the opening of a spin gap. In the 2D case Emery, Kivelson, and Lin[15] discussed phase separation in the large-J region. For 1D, we can also expect such a phase separation. First, we discuss the parameter regime in which it takes place and then estimate the correlation exponent in the remaining region.

The Lanczos method is used to obtain the energies of the ground state and a few low-lying excited states. By examining the convergence of the energy levels, we confirm that the lowest five levels are accurately determined (about 6 decimals). Figure 1(a) shows the ground-state energy as a function of electron density n in sixteen sites for values of J from 0 to 4. In order to achieve systematic convergence to the thermodynamic limit, we choose periodic boundary conditions for $N=4m+2$ and antiperiodic boundary conditions for $N=4m$, with N being the electron number and m an integer. This removes accidental degeneracies so that the ground state is always a singlet with zero total momentum as for the large-U Hubbard model.[5] We confirm this analytically at $J=2$ and numerically for any J. The finite-size curvature of the energy changes sign for $2.8<J<3.6$, indicating that phase separation takes place in this region.

To estimate the boundary more precisely, we calculate the finite-size equivalent of the compressibility

$$\kappa=\frac{N_a}{N^2}\Big/\left(\frac{E(N+2)+E(N-2)-2E(N)}{4}\right), \quad (2)$$

where $E(N)$ is the ground-state energy with N electrons on N_a sites ($n=N/N_a$). This expression gives the true thermodynamic compressibility unless a many-electron bound state is formed. This is clearly not the case in the TL part of the phase diagram. We show in Fig. 2 the values of J_c at which $1/\kappa$ crosses zero for $N_a=10,12,16$.

In order to check the convergence, we compare the sixteen-site results with the thermodynamic limit at the solvable cases $J=0$ and 2. As shown in Fig. 3, the compressibility becomes a well-converged quantity if we

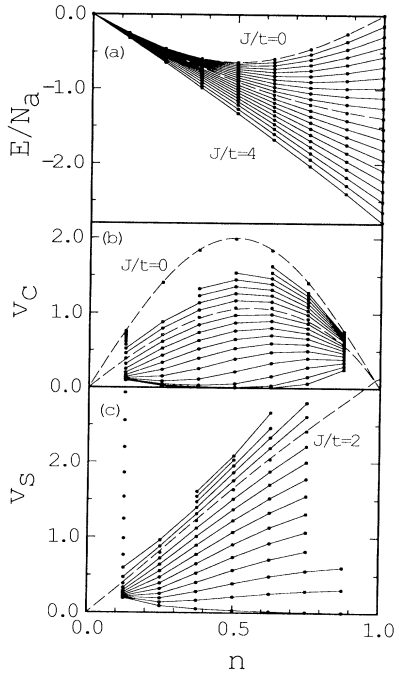

FIG. 1. (a) Total energy, (b) charge velocity, and (c) spin velocity as a function of electron density in sixteen sites for various values of J. Dashed lines indicate the quantities in the thermodynamic limit for $J=0$ and $J=2$.

use Eq. (2) and the boundary conditions defined above. Note that $1/\kappa$ becomes zero in the phase-separated region in the thermodynamic limit, because we calculate the true ground-state energy. Therefore, apart from finite-size effects, J_c gives an accurate estimate of the boundary. Complementary estimates of J_c can be obtained using the Maxwell construction, and they are also shown in Fig. 2. Taking into account the error bars on these calculations due to the finite-size effect, the two sets of estimates are in good agreement. We emphasize that the essential features of the phase diagram are clearly established. The slope of the line of phase separation indicates that separation occurs between the empty phase ($n=0$) and a low-density phase. The latter could be a state consisting of weakly bound electrons. This behavior is consistent with a recent perturbative calculation with respect to t/J (Ref. 16) and with the results of a recent Monte Carlo calculation by Assaad and Würtz. A detailed comparison of the Monte Carlo results with Fig. 2 will be published elsewhere.[17]

Emery, Kivelson, and Lin[15] discussed phase separation in the 2D case. In 1D it is possible to show, using simple lower and upper bounds on the energy, that the total energy, at least for $J>8$, is asymptotically linear in the total electron number, $E(N)=-NJ\ln 2$, i.e., in the 1D Heisenberg energy per site. This means that in the large-J region, the ground state at a given density is a Heisenberg chain island ($n=1$) and an empty phase ($n=0$). As J is decreased there are three simple ways of

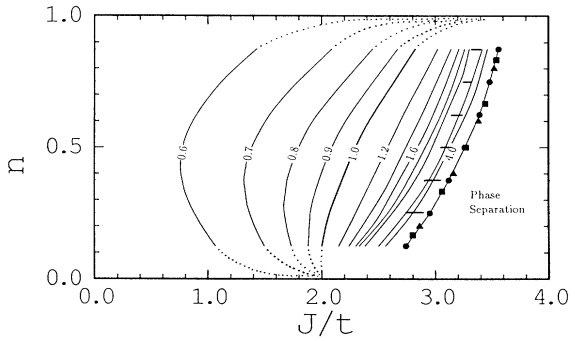

FIG. 2. Phase diagram of the 1D t-J model determined from the sixteen-site cluster calculation. The curves show the contours of constant correlation exponent K_ρ. They are calculated from a mesh of points similarly spaced in density in steps of $0.2J$. Solid symbols show the values where the inverse compressibility crosses zero for 10 (triangles), 12 (squares), and 16 (circles) sites, representing the boundary of the phase separation. An alternative estimate of the boundary is obtained by the Maxwell construction. In this criterion phase separation takes place between $n=0$ and the critical value of n, n_c, at which $E(N)/N$ has a minimum. Solid bars represent the region of J where $E(N)/N$ is minimum for each electron density in the sixteen sites.

destroying the fully phase-separated state. For intermediate J, phase separation can survive with an electron-rich phase with $n\sim 1$ and/or a hole-rich phase with $n\sim 0$. For example, in the spinless fermion model with attractive interaction (t-V model), phase separation disappears abruptly for all densities at a critical value of the interaction ($V/t=2$).[18] Alternatively, either phase separation is destroyed first in the low-density limit ($n\sim 0$) or in the limit of small doping ($n\sim 1$). In the following we discuss these two possibilities.

In the first case, we estimate the critical value of J using the argument of Emery, Kivelson, and Lin.[15] Consider the state with complete phase separation and let two electrons evaporate from the Heisenberg chain, forming a singlet bound state in the region $J>2$. (Note

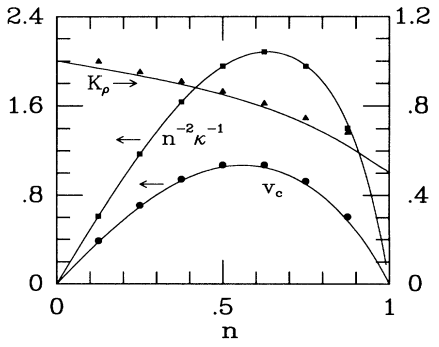

FIG. 3. Results for sixteen sites compared with the asymptotic result (200 sites) for the inverse compressibility (squares), charge velocity (circles), and the resulting exponent (triangles).

that phase separation takes place much above $J=2$.) The loss of energy due to breaking two bonds is $+2J\ln 2$, while the gain of energy is $-J-4t^2/J$. The latter is obtained exactly by solving the two-electron problem for the infinite chain. Considering the energy balance, we obtain $J_c=2/\sqrt{2\ln 2-1}=3.22$. As pointed out by Emery, Kivelson, and Lin, this variational estimate would be exact if there were no bound states with more than two particles. Note that within this assumption, the discontinuity of the second derivative of the two-particle energy with respect to J leads to a second-order phase transition at $J=2$ for $n\sim 0$.

In the second case, we have to balance the gain in kinetic energy with the loss of exchange energy due to inserting two holes in a Heisenberg chain. We calculate the ground-state energy with N_a-2 electrons in N_a sites relative to the Heisenberg energy in N_a-2 sites. This energy becomes negative for $J<3.14$, 3.30, and 3.34 for $N_a=8$, 12, and 16, respectively. Although a small size dependence remains, we estimate $J_c(n=1)=3.5$ which is greater than the estimate obtained previously from the two-particle instability. This means that the fully phase-separated state is destroyed first by introducing holes in the Heisenberg chain. In this case the empty phase with $n=0$ remains as one of the two components. This is consistent with the phase boundary in Fig. 2 derived from the calculation of the compressibility. Note that this situation is the opposite of that discussed by Emery, Kivelson, and Lin[15] for the 2D t-J model.

Next we estimate the correlation exponent of the TL liquid in the remaining parameter region. To support the statement that the system behaves as a TL liquid, we calculate the central charge c which characterizes the universality class of the model. In the TL liquid $c=1$ as shown rigorously for the Hubbard model[10] and the t-J model at $J=2$.[14] We obtain c by fitting the ground-state energy as $E/N_a=\epsilon_\infty-\pi(v_c+v_s)c/6N_a^2$ at $n=0.5$ in the clusters with $N_a=4$, 8, 12, and 16. Here the charge and spin velocities, v_c and v_s, are determined from the excited states of the sixteen-site diagonalization as discussed below. We find that c is almost constant ($c\sim 1.01$) in the region $J=1.0-3.0$ where both v_c and v_s can be calculated accurately. This confirms that no other instability occurs at this density and the system behaves as a TL liquid before phase separation. In fact, a spin gap opens at very low density, but we discuss this instability later. In the region $J>3.4$, the size dependence of the ground-state energy differs from the above formula, and this is consistent with the phase boundary.

To estimate the exponent we use the relation

$$\frac{1}{n^2\kappa}=\frac{\pi}{2}\frac{v_c}{K_\rho}, \tag{3}$$

which holds generally in the TL liquid[8-10] where K_ρ is related simply to all the correlation exponents: For example, the charge-charge correlation decays as e^{4ik_Fr}/r^{4K_ρ} and the superconducting correlation decays as $1/r^{1+1/K_\rho}$ with k_F being the Fermi wave number of the noninteracting system.[2] To check the reliability of the estimated values for v_c and K_ρ in the sixteen-site cluster, we study the size dependence at the solvable case ($J=2$). We solve numerically the Lieb-Wu-type coupled equations for finite systems in Sutherland's formulation.[11] Since one of the sets of quantum numbers (I_j) represents the charge degrees of freedom, the lowest charge excitation with momentum $2\pi/N_a$ is obtained by replacing the largest I_j by I_j+1. The charge velocity is calculated as $v_c=(E_1-E_0)/(2\pi/N_a)$ with E_1-E_0 being the charge excitation energy. The comparison between the sixteen-site result and the thermodynamic limit is summarized in Fig. 3. The quantities v_c and K_ρ converge smoothly to their value in the thermodynamic limit. The maximum error in K_ρ is less than 5%.

In order to identify which one of the energy levels in the exact diagonalization corresponds to the lowest charge excitation we compare the energies with E_1 at $J=2$. Then we follow that energy level to obtain the charge velocity as a function of J. Figure 1(b) shows v_c derived in this way for various values of J. At $J=0$, it is known exactly that $v_c=2\sin(2k_F)$, because the system behaves as a gas of spinless fermions. Since the spin degeneracy is lifted in the small-J region and there are many low-lying states proportional to J, it is difficult to identify the energy level corresponding to the lowest charge excitation in this region. However, we can easily calculate v_c in the most interesting region ($J>1$). v_c decreases monotonically as J increases. Similarly the spin velocity can be obtained and is shown in Fig. 1(c). At $J=0$, it should be zero. Although there is a large size dependence in the low-density region, it is clear that v_s increases with J and should be zero in the low-density limit for $0<J<2$.

Substituting the obtained charge velocity and compressibility in Eq. (3), we plot the correlation exponent K_ρ in Fig. 2. Note that K_ρ has a 5% error at $J=2$, as shown in Fig. 3. This finite-size effect causes an error of $\Delta J\sim 0.2$. But the global features of the phase diagram are not changed and are consistent with the expectations of Haldane.[19] Recently Assaad and Würtz obtained $K_\rho=1.0\pm 0.3$ at $J=2.2$ and $n=0.5$ which compares favorably with Fig. 2. The exponent K_ρ takes the value $\frac{1}{2}$ in the limiting cases $J=0$ for all densities, $n\to 1$ for all J, and $n\to 0$ for $J<2$ above which the two-particle bound state is formed. All contours for $K_\rho\leq 1$ should connect the two critical points $J_c\sim 3.5$, $n=1$ and $J=2$, $n=0$. Indeed, in the low-density limit for $J<2$, all the curves seem to converge to $J=2$ and $n=0$. However, above $J=2$ it is difficult to determine the phase diagram precisely, because K_ρ increases rapidly near the singular region. In the high-density limit ($n\sim 1$), all the curves cross the line $J=2$ and tend to converge to one point J_c ($n=1$). The most interesting result of this phase diagram is that there is a finite region with $K_\rho>1$ between $J=2$ and the boundary of phase

separation. According to the g-ology,[2] $K_\rho > 1$ implies that the superconducting correlation is the most divergent ($g_2 < 0$). This is consistent with recent quantum Monte Carlo simulations.[17,20]

As suggested by Haldane[19] a spin gap can open in the low-density region for $J > 2$, if a gas of singlet bound electron pairs is formed. We investigated this possibility by extrapolating the energy of four electrons to the infinite-size limit using the exact energies up to 113 sites for $J = 2.0$–4.0. Indeed, the estimated energy coincides with twice that of the singlet bound state of two electrons (i.e., $-2J - 8/J$) for $J = 2.0$–2.95 with an accuracy of $10^{-4}t$, above which a four-electron bound state takes place. This shows that a gas of singlet bound pairs is realized in the low-density region for $J = 2.0$–2.95. To put an upper bound on this phase, we study the spin susceptibility χ_s. When a spin gap opens χ_s converges to zero. We calculate χ_s from the energy difference ΔE between the ground state and the lowest $S = 1$ state as $\chi_s = (2N_a \Delta E)^{-1}$ at $n = \frac{1}{3}$ for $N_a = 6$, 12, and 18. Analyzing the size dependence, we found no evidence for a spin gap at this electron density so that the singlet phase is restricted to the very-low-density regime. Further calculations are in progress to clarify the phase diagram in the spin-gap region and will be published elsewhere. It is also possible to have other phases between the singlet pair gas and phase separation, such as a gas of four-electron bound states. From the above analysis, however, the region of such large-molecule phases would be very small in the space of (J,n) variables.

In conclusion, we have established the phase diagram of the 1D t-J model. Although the detailed structure around $n = 0$ and $J = 2$ requires a little further investigation, the global features are reliable. The fully phase-separated state at large J is destroyed by dissolving holes into the Heisenberg chain. In the remaining region, we have calculated the correlation exponent of the TL liquid. In the vicinity of phase separation, we have found a region where the superconducting correlation is the most divergent. In the low-density region and just before phase separation, we find a phase of singlet bound electron pairs. The richness of the phase diagram is remarkable.

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