# Phase Diagram of the One-Dimensional *t-J* Model from Variational Theory

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We study a class of variational wave functions for strongly interacting one-dimensional lattice fermions in which correlations among the particles are specified by a single variational parameter. We find that the wave functions describe the ground-state properties of the one-dimensional $t$-$J$ model remarkably well over the entire phase diagram in which interaction strength and density are varied. Specifically the wave function describes a Tomonaga-Luttinger liquid at low $J/t$, a phase-separated state at large $J/t$, and a stable state with infinite compressibility between these phases at low densities.

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The $t$-$J$ model was originally introduced to describe the motion of holes doped into a Mott insulating state [1-3]. The model is nontrivial even in one dimension, and it is important to develop a complete description of its phase diagram. The 1D $t$-$J$ Hamiltonian is written in the subspace of no doubly occupied sites as

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

The model is exactly solvable only at $J/t=0$, where it is equivalent to the $U=\infty$ Hubbard model, and $J/t=2$ [4,5]. In both of these cases the ground state belongs to a general class of interacting Fermi systems known as Tomonaga-Luttinger (TL) liquids, which exhibit power-law singularities in the momentum distribution at the "Fermi surface" [6,7]. Additionally, at large $J/t$ the attractive interaction term dominates the kinetic energy and the model phase separates in order to optimize the Heisenberg exchange energy in (1).

To obtain the complete phase diagram of the model, approximations must be used at other values of $J/t$. For example, Ogata *et al.* [8] have applied exact diagonalization to small systems to investigate the phase diagram. They find that indeed the model behaves as a TL liquid for all values of $J/t$ below the critical value for phase separation and have hypothesized that a third phase of bound singlet pairs may separate the other phases at very low density.

In this paper we use a variational technique to investigate the ground-state properties of the $t$-$J$ model. This method is approximate, as we are limited by our variational subspace, but we are able to work with much larger systems and can practically eliminate finite-size effects. We find our results are remarkably reliable where comparison with exact results is possible, and we find some important differences with previous numerical work elsewhere in the phase diagram.

We study a variational many-fermion state constructed from a Jastrow-Slater wave function

$$\Psi(r_i^{\uparrow},r_i^{\downarrow}) = |F(r_i^{\uparrow},r_i^{\downarrow})|^{\nu}P_dS(r_i^{\uparrow})S(r_i^{\downarrow})\,, \qquad (2)$$

where $S(r_i)=\text{Det}[e^{ik_jr_i}]$ is a Slater determinant of single-particle plane-wave states and $P_d=\prod_i(1-n_{i\uparrow}n_{i\downarrow})$ projects out all states with doubly occupied sites. We restrict ourselves in this work to a spin singlet and therefore have equal numbers of up and down electrons in the Slater factor.

The Jastrow factor $|F(r_i^{\uparrow},r_i^{\downarrow})|^{\nu}$ in (2) uses the modulus of a Slater determinant in *all* electron coordinates to correlate the particles [9,10]. This factor is manifestly symmetric under all permutations, thus preserving the spin-singlet nature of the unmodified state. A positive value of the variational parameter $\nu$ induces a smooth correlation hole between all particles. Classically, $\nu$ specifies the effective temperature or strength of these correlations. On the other hand, a negative $\nu$ induces an attractive correlation between particles which competes with the Pauli repulsion in the ground state. Ultimately, for sufficiently negative $\nu$, this attraction overcomes the statistical repulsion, and phase separation occurs.

The nature of the wave function for various values of $\nu$ can be studied quantitatively by mapping it onto a classical two-component hard-core gas with logarithmic interactions [3]. The modulus of (2) can be rewritten with the projector omitted as

$$|\Psi| = \prod_{i<j}\exp(-\beta V_{ij})\,, \qquad (3)$$

where $V_{ij}=-(1/\beta)(\nu+\frac{1}{2}+\frac{1}{2}\sigma_i\sigma_j)\ln|z_i-z_j|$. Here $z_i=\exp(I\Delta kr_i)$ with $\Delta k=2\pi/L$ for a system of $L$ sites and $\sigma_i=\pm1$ is the spin index. Positive values of $\nu$ correspond to an additional repulsive interaction while negative values are attractive. For $\nu<-\frac{1}{2}$ the average interaction is attractive, and the system phase separates.

We use the variational quantum Monte Carlo method to evaluate the energy and other observables using the wave function (2) [11-13]. With a determinantal Jastrow factor, it is simple to calculate the derivative of any observable with respect to $\nu$ directly, which greatly helps determination of the optimum $\nu$ for a given value of $J/t$. In previous work [10] we found that for $J=0$, the optimum value of this variational parameter ranges from $\nu=1$ at low densities to $\nu=0.5$ close to half filling. At

 

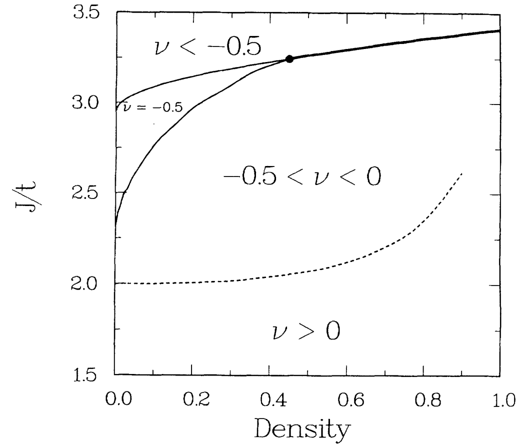


FIG. 1. The phase diagram of the $t$-$J$ model as determined by our variational wave function. The phase-separated state is marked by $\nu < -0.5$, and other regions display the appropriate range of $\nu$. At densities above $n \approx 0.45$, the transition to phase separation has a discontinuous jump in $\nu$ shown by the thick solid line. At lower densities, $\nu = -0.5$ for a range of $J/t$ before phase separation occurs. The dashed line shows where $\nu = 0$, the Gutzwiller wave function. All systems contained at least 100 electrons and 20 holes. Points beyond $n = 0.9$ are extrapolated.

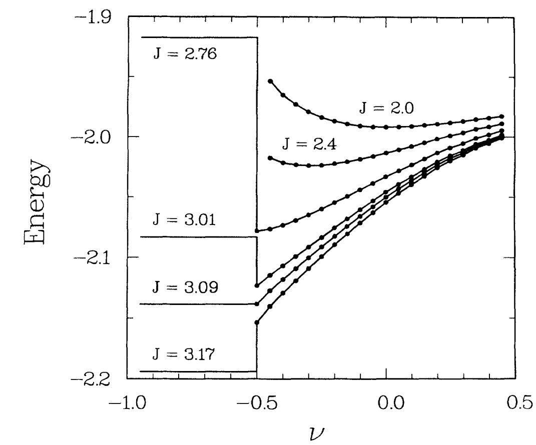


FIG. 2. The energy as a function of variational parameter $\nu$ for various values of $J/t$ for 150 particles on 1500 sites. The optimum $\nu$ decreases continuously with increasing $J$ for $J/t \lesssim 2.76$. Once $\nu = -\frac{1}{2}$ is reached, this value remains the minimum for $2.76 \lesssim J/t \lesssim 3.09$. Values for $\nu < -\frac{1}{2}$, the phase-separated state, are extrapolated to the infinite-system limit to remove edge effects and thus are constant. This regime is the minimum for $J/t \gtrsim 3.09$.

quarter filling ($n = 0.5$), $\nu = 0.75$.

The phase diagram of the $t$-$J$ model as determined by our wave function is shown in Fig. 1. We see that three distinct phases occur. For $\nu > -\frac{1}{2}$ the system behaves as a TL liquid with a power-law singularity in the momentum distribution at the Fermi surface. In this range, we find that for $\nu > 0$ spin correlations dominate the long-range behavior of the system, while for $\nu < 0$ singlet pairing correlations dominate, in agreement with TL theory [8,14]. The dashed line shows where the variational parameter passes through $\nu = 0$ and (2) reduces to the Gutzwiller wave function. This line converges to $J/t = 2$ at low densities and remains relatively close to this point over a broad range of densities. It has been shown independently [15] that the Gutzwiller wave function is an excellent trial wave function at $J/t = 2$.

For $\nu < -\frac{1}{2}$ the wave function (2) describes a spatial condensation of the particles on the chain. The Jastrow factor serves merely to bind the particles—the kinetic energy vanishes while the spin dynamics are described by the remaining part of the wave function, namely, the Gutzwiller-projected Fermi sea, which is well known to give an excellent approximation to the exact Heisenberg ground state [3,16].

The boundary between these two regions is interesting. For densities above $n \approx 0.45$, there is a first-order transition in which $\nu$ jumps discontinuously to the phase-separated $\nu < -\frac{1}{2}$ region. However, at lower densities $\nu$ decreases with increasing $J$ to $\nu = -\frac{1}{2}$ and then remains there over a finite range of $J/t$ before phase separation occurs. We find two second-order lines bounding this $\nu = -\frac{1}{2}$ phase which terminate at a tricritical point at $n \approx 0.45$. Figure 2 shows this behavior in more detail with a plot of energy as a function of $\nu$ for various values of $J/t$ at density $n = 0.1$. Starting from small $J/t$, the energy minimum moves to lower $\nu$ as $J$ increases. The optimized exponent remains at $\nu = -\frac{1}{2}$ over the range $2.76 \lesssim J/t \lesssim 3.09$, beyond which the phase-separated state ($\nu < -\frac{1}{2}$) becomes the ground state. In the phase-separated state, the energy is independent of $\nu$ in the infinite-system limit, and the energy contours for $\nu < -\frac{1}{2}$ are flat.

Exactly at $\nu = -\frac{1}{2}$ we can write the wave function (2) as

$$\Phi = \prod_{i<i'} (z_i - z_{i'}) \prod_{j<j'} (z_j - z_{j'}) \prod_{k<k'} |z_k - z_{k'}|^{-1/2} \prod_k z_k^{-(N-1)/2}, \tag{4}$$

where the $i$'s ($j$'s) span the $N$ up (down) electrons, and the $k$'s span all electrons. In this form we see the wave function closely resembles the semion wave function gauged to the fermion representation which was studied in several recent two-dimensional problems [17,18]. From the classical gas analogy one may conclude that the compressibility of this phase is infinite; we examine this property in more detail below.

Correlation functions obtained from (2) are shown in Fig. 3. For positive $\nu$, or small $J/t$, the spin-correlation function exhibits a sharp cusp at $2k_F$, indicating that spin correlations at $2k_F$ are dominant at long length scales. As $\nu$ decreases

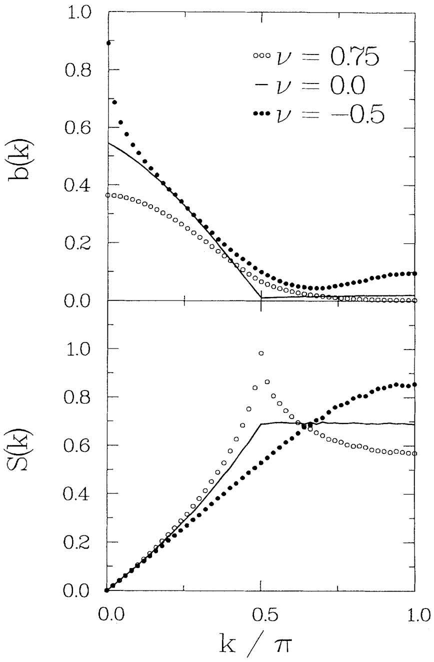


FIG. 3. The spin and superconducting correlation functions for various values for $\nu$ for the quarter-filled band. The cusp in $S(k)$ at $2k_F=\pi/2$ is suppressed as $\nu$ decreases while the $k=0$ pairing cusp is enhanced. The system contains 50 electrons on 100 sites.

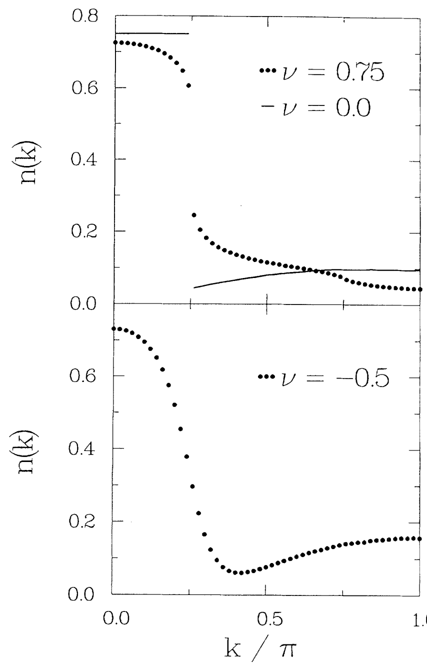


FIG. 4. The momentum distributions for the quarter-filled band. The power-law singularity at $k_F=\pi/4$ steepens as $\nu$ approaches $\nu=0$ from both the positive and negative sides, and there is a true discontinuity at the Fermi level only at $\nu=0$.

with increasing $J$, this cusp is suppressed while a cusp at $k=0$ is enhanced for correlations of the pair amplitude. These dominate for $\nu<0$. All correlation functions in this problem can be characterized by the single quantity $K_\rho$ [19–21]. Specifically, the spin and superconducting pair-correlation functions decay asymptotically as

$$\langle S_z(r)S_z(0)\rangle \sim A_1 r^{-2} + A_2\cos(2k_F r)r^{-(1+K_\rho)},$$

$$\langle b^\dagger(r)b(0)\rangle \sim B_1 r^{-(1+1/K_\rho)} + B_2\cos(2k_F r)r^{-(K_\rho+1/K_\rho)},$$

where $b(r)=(1/\sqrt{2})(c_{r\uparrow}c_{r+1\downarrow}-c_{r\downarrow}c_{r+1\uparrow})$. We find that decreasing $\nu$ corresponds to increasing $K_\rho$, with the $\nu=0$ (Gutzwiller) state having $K_\rho=1$, the value at which spin and pair correlations have equal strength. Additionally, $K_\rho(\nu=0.75)\approx 0.43$ and $K_\rho(\nu=-0.5)=\infty$. The latter value was obtained from finite-size scaling of the $k=0$ pairing cusp and confirms the infinite compressibility of the special $\nu=-\frac{1}{2}$ state [14].

Finally, the momentum distributions are shown in Fig. 4. In the TL regime, the momentum distribution exhibits a power-law singularity near $k_F$ of the form

$$n(k)=n(k_F)-C|k-k_F|^\alpha \operatorname{sgn}(k-k_F),$$

where $\alpha=\frac{1}{4}(K_\rho+1/K_\rho-2)$. At $\nu=0.75$ it shows a singularity with $\alpha\approx 0.19$ at $k_F$. This singularity sharpens and evolves into a discontinuity exactly at $\nu=0$, and then decays again for negative $\nu$. For $\nu=-0.5$, $\alpha=\infty$ and $n(k)$ is analytic at the Fermi surface.

In conclusion, we have introduced a variational wave function that allows us to explore the ground-state properties of the $t$-$J$ model on the one-dimensional lattice. We find a first-order phase transition between a correlated "metallic" state and the phase-separated state with increasing $J/t$ at high densities, while at low densities we obtain a third condensed state with infinite compressibility. The detailed nature of the spin correlations in this third phase is interesting. It has been suggested that a spin gap appears in this phase, but the present treatment is not able to confirm this possibility. We actually observe a linear spin structure factor at small $k$ in Fig. 3 for all $\nu$, indicative of a *gapless* spin-liquid state. We are presently working to expand our variational space to check for instabilities in this region.

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[1] P. W. Anderson, Science **235**, 1196 (1987).

[2] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).

[3] C. Gros, R. Joynt, and T. M. Rice, Phys. Rev. B **36**, 381 (1987).

[4] M. Ogata and H. Shiba, Phys. Rev. B **41**, 2326 (1990).

[5] N. Kawakami and S.-K. Yang, Phys. Rev. Lett. **65**, 2309 (1990).

[6] J. Sólyom, Adv. Phys. **28**, 201 (1979).
[7] F. D. M. Haldane, J. Phys. C **14**, 2585 (1981); Phys. Rev. Lett. **45**, 1358 (1980).
[8] M. Ogata, M. Luchini, S. Sorella, and F. F. Assaad, Phys. Rev. Lett. **66**, 2388 (1991).
[9] C. S. Hellberg and E. J. Mele, Phys. Rev. B **44**, 1360 (1991).
[10] C. S. Hellberg and E. J. Mele, Int. J. Mod. Phys. (to be published).
[11] C. Gros, Ann. Phys. (N.Y.) **189**, 53 (1989).
[12] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **56**, 1490 (1987); **56**, 3570 (1987); **56**, 3582 (1987); **57**, 2482 (1988); **59**, 3669 (1990).
[13] D. Ceperley, G. V. Chester, and M. H. Kalos, Phys. Rev. B **16**, 3081 (1977).
[14] F. F. Assaad and D. Würtz, Phys. Rev. B **44**, 2681 (1991).
[15] H. Yokoyama and M. Ogata (to be published).
[16] F. Gebhard and S. Vollhardt, Phys. Rev. Lett. **59**, 1472 (1987); Phys. Rev. B **38**, 6911 (1988).
[17] S. M. Girvin, A. H. MacDonald, M. P. A. Fisher, S.-J. Rey, and J. P. Sethna, Phys. Rev. Lett. **65**, 1671 (1990).
[18] E. J. Mele, G. Segré, and C. Bruder, Phys. Rev. B **43**, 5576 (1991).
[19] H. Frahm and V. E. Korepin, Phys. Rev. B **42**, 10553 (1990).
[20] H. J. Schulz, Phys. Rev. Lett. **64**, 2831 (1990).
[21] Y. Ren and P. W. Anderson (to be published).