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Luttinger-liquid instability in the one-dimensional t-J model

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We study the t-J model in one dimension by numerically projecting the true ground state from a Luttinger-liquid trial wave function. We find the model exhibits Luttinger-liquid behavior for most of the phase diagram in which interaction strength and density are varied. However, at small densities and high interaction strengths a new phase with a gap to spin excitations and enhanced superconducting correlations is found. We show this phase is a Luther-Emery liquid and study its correlation functions.

The t-J model was proposed to describe the dynamics of holes doped into a Mott insulating state.[1–3] Even in one dimension, determining the complete phase diagram for this apparently simple model has proven to be quite formidable, and the ground-state structure turns out to be far richer than initially suspected. In this paper we combine a variational approach with an exact ground-state projection method to study the properties of this model.

The Hamiltonian for the t-J model in one dimension can be written in the subspace of no doubly occupied sites as

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

The model has been solved exactly only for $J \to 0$, where it is equivalent to the $U \to \infty$ Hubbard model, and $J = 2t$.[4,5] In both cases the ground state at arbitrary density belongs to a broad class of interacting Fermi systems known as Luttinger liquids, which exhibit power-law decay of correlation functions with exponents characterized by a single parameter.[6–8] Additionally, for very large J/t the attractive Heisenberg interaction term in (1) dominates the kinetic energy and the model phase separates.

To obtain the rest of the phase diagram of the t-J model, several numerical approaches have been used. For example, Ogata *et al.*[9] have exactly diagonalized this Hamiltonian on a 16-site ring and find the model behaves as a Luttinger liquid for all values of J/t below a critical value at which phase separation occurs. They hypothesized that a third phase of bound singlet pairs may separate the other phases at very low density but were unable to resolve this phase with such small system sizes.

In this paper we employ a Luttinger-liquid variational wave function to approximate the ground state of the one-dimensional t-J model[10–13] and then use a numerical projection technique to extract the true ground state from this trial state. With these methods, we can accurately investigate much larger systems than attainable by previous techniques. We confirm that the t-J model has a Luttinger-liquid ground state for most of its uniform density phase diagram, and in this region the ground state is well described by the trial state. At small densities, however, we find a third phase separating the Luttinger-liquid and phase-separated states. This phase behaves as a Luther-Emery liquid, exhibiting a gap to spin excitations and enhanced superconducting correlations.

In previous work[12] we studied the ground state with a Luttinger-liquid trial state written in the subspace of no doubly occupied sites as a Jastrow-Slater wave function

$$\Psi_\nu = \prod_{i<j}|d_{ij}|^{\nu}\ S(r_i^{\uparrow})S(r_i^{\downarrow}), \quad (2)$$

where $S(r_i) = \mathrm{Det}[e^{ik_jr_i}]$ is a Slater determinant of single-particle plane wave states and $d_{ij} = \sin[\pi(r_i - r_j)/L]$ for a system of size L. The Jastrow factor $\prod_{i<j}|d_{ij}|^{\nu}$ in (2) modulates the wave function by the distance between all pairs of particles raised to the power ν, taken as a single variational parameter. Positive values of ν induce a smooth correlation hole between all particles, while negative values provide an attractive correlation competing with the Pauli repulsion. For $\nu < -1/2$ this attraction overcomes the statistical repulsion, and phase separation occurs. The long-range nature of this Jastrow factor generates the Luttinger-liquid behavior of the wave function.[13,14] This wave function has been considered in two dimensions where it also exhibits an algebraic singularity at the Fermi surface.[15,16]

Applying (2) to the t-J model one finds the optimum value of the variational parameter ν varies continuously with interaction strength and density over most of the phase diagram prior to the critical J/t for phase separation. However, at small densities we found a third region separating the Luttinger-liquid and phase-separated states where the optimized parameter is pinned at the critical state $\nu = -1/2$. At this point the many-body system in the trial subspace has infinite compressibility, which physically cannot extend for a range of interaction strengths. One concludes that the true ground state here likely lies far from our variational subspace. We would like a systematic way of both checking the accuracy of the trial state where we think it is doing well and determining the exact ground state in this third region.

In this work, we start with the optimized trial state (2) and project it onto the exact ground state

numerically.[17–20] A series of increasingly accurate approximants to the ground state is generated by $|p\rangle = (H - W)^p|\Psi_\nu\rangle$, where H is the Hamiltonian and W is a numerical constant. These states approach the true ground state for large p provided $|E_0 - W| > |E_i - W|$ for all excited states E_i. For the t-J model with $J > 0$ we may choose $W = 0$. In principle this method can be used to project any trial state not orthogonal to the ground state, but good initial states give faster convergence and smaller statistical errors.

To evaluate ground-state expectation values of an arbitrary operator, we calculate

$$\langle O_p\rangle = \frac{\langle p|O|p\rangle}{\langle p|p\rangle} = \frac{\langle\Psi_\nu|H^pOH^p|\Psi_\nu\rangle}{\langle\Psi_\nu|H^{2p}|\Psi_\nu\rangle} \tag{3}$$

and take the large p limit. For sufficiently large powers, the scaling of (3) is dominated by the contribution from the first excited state overlapping the trial state. Thus we can write

$$\langle E_p\rangle = E_0 + \delta\exp(-2\Delta p) + \cdots \tag{4}$$

with $\exp(-\Delta) = |E_1 - W|/|E_0 - W|$. An operator not commuting with the Hamiltonian has an additional cross term:

$$\langle O_p\rangle = O_0 + \delta_1\exp(-\Delta p) + \delta_2\exp(-2\Delta p) + \cdots. \tag{5}$$

We use the convergence of the energy (4) to fix Δ, and then use (5) to determine the ground-state values of the rest of the observables.

Traditionally (3) has been calculated using a hybrid of two numerical techniques. First the trial wave function Ψ is sampled with variational Monte Carlo to give an ensemble of initial configurations $|\alpha\rangle$.[3,21,22] Then for each $|\alpha\rangle$ the product H^p is sampled stochastically using a method similar to the Neumann-Ulam matrix method.[23] The products are sandwiched to evaluate $\langle H^pOH^p\rangle$ and the normalization $\langle H^{2p}\rangle$. This approach throws away much information, specifically the details of the intermediate states in the evaluation of each H^p.

We developed a much more efficient algorithm for evaluating (3) by combining the two operations. In usual variational Monte Carlo a new configuration $|\beta\rangle$ is chosen from a previous configuration $|\alpha\rangle$ with probability

$$P^{\rm VMC}_{\alpha\to\beta} = \min\left(1, \left|\frac{\Psi_\beta}{\Psi_\alpha}\right|^2\right). \tag{6}$$

After many transitions, this leads to a distribution of configurations proportional to $|\Psi_\alpha|^2$. If new configurations are instead chosen with the probability

$$P_{\alpha\to\beta} = \frac{1}{z_\alpha}\frac{\Psi_\beta}{\Psi_\alpha}H_{\beta\alpha} \tag{7}$$

with

$$z_\alpha = \sum_{\beta'}\frac{\Psi_{\beta'}}{\Psi_\alpha}H_{\beta'\alpha}, \tag{8}$$

the distribution for a configuration $|\alpha\rangle$ approaches $|\Psi_\alpha^2/z_\alpha|$. This method of generating new initial configurations is the same used to evaluate the products H^p, so the calculation of the initial states $|\alpha\rangle$ and the series of new states $|p\rangle = H^p|\alpha\rangle$ can be combined.

The algorithm improves on the traditional approach in two ways. When evaluating a diagonal expectation value, such as $\langle n(r)n(0)\rangle$ or $\langle S_z(r)S_z(0)\rangle$, our method evaluates a new $\langle\Psi_\beta|H^pOH^p|\Psi_\alpha\rangle$ at every step of the random walk, so calculations of different powers p require the same amount of time. Additionally, for any expectation value, an arbitrary number of different values of p may be calculated in parallel. The only disadvantage of our approach is that ergodicity is violated as $J \to 0$, and the old method must be used in this limit. Both methods offer an improvement to Green's function Monte Carlo in that exact correlation functions can be calculated.[24] Since statistical errors grow with increasing p, we generally chose the maximum power to be ten times the system size.

The phase diagram of the t-J model determined by our projection technique is shown in Fig. 1. We see that three distinct phases occur. For small J/t, the ground state is a Luttinger liquid with spin correlations dominating the long-range behavior. Increasing J suppresses these correlations, and the ground state passes through the Fermi-liquid point of the Luttinger-liquid spectrum at the dashed line. Above this line the Luttinger liquid has dominant singlet pairing correlations, and for very large J/t the ground state is phase separated.[9,12,25,26]

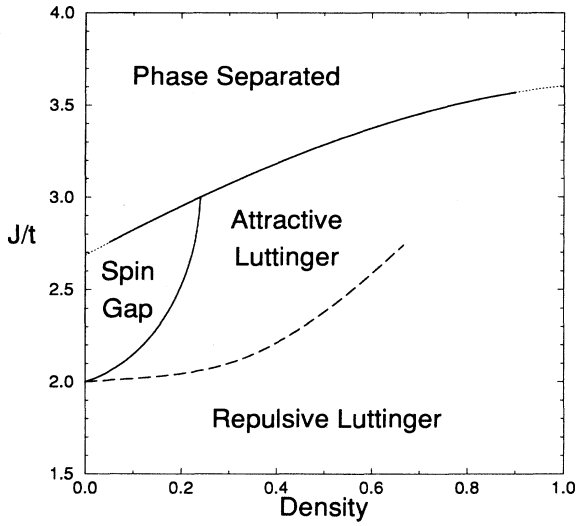

FIG. 1. The phase diagram of the t-J model as determined in this paper. The Luther-Emery state is the region labeled "Spin Gap." The dashed line indicates $K_\rho = 1$, the Fermi-liquid phase. Below this line the Luttinger liquid has dominant antiferromagnetic correlations, while above this line singlet pair correlations decay with the smallest exponent. The phase separation boundary is determined by the divergence of $n(k \to 0)$, the lower Luther-Emery boundary by the behavior of $S(k \to 0)$, and the Fermi-liquid line by $S(k \to 2k_F)$. All systems contained at least 100 sites and ten electrons and holes, so phase boundaries cannot extend to the extreme densities. The dotted lines are extrapolations.

As will be reported in detail elsewhere, in the Luttinger-liquid regime the trial state (2) approximates the exact ground state very well.

In this work we see clear evidence of a new Luther-Emery-liquid phase (labeled "Spin Gap" in Fig. 1) separating the Luttinger-liquid and phase-separated states at small densities.[27,8] Unlike all Luttinger states, this new phase exhibits short-range spin correlations, and thus a gap to spin excitations, while both charge and singlet pair correlations decay algebraically. Physically one can view the Luther-Emery liquid as a translationally invariant coherent quantum fluid of bound singlet pairs. The pairs are correlated and can be treated at a simple level as an interacting fluid of hard-core bosons.

Luther-Emery states have been observed in diluted spin models that exhibit gaps in the saturated state, such as the t-J model with Ising anisotropy[28] or the next-nearest-neighbor t-J model.[29] Additionally this phase is present in the t-J-V model at quarter filling[30]. This work provides the clearest evidence to date of the spontaneous formation of a Luther-Emery state by doping a gapless parent state.

A sample spin correlation function in the Luther-Emery phase is plotted in Fig. (2) with the correlation function obtained from the unprojected trial state shown for comparison. The variational function exhibits the linear behavior at small wave vectors characteristic of Luttinger liquids, while the exact function is quadratic at small k and analytic at all wave vectors, consistent with exponentially decaying spatial correlations. We calculate the boundary between the Luttinger and Luther-Emery states by the crossover from linear to quadratic behavior at small wave vectors.

More definitive evidence of Luther-Emery behavior can be seen in the superconducting correlation function plotted in Fig. 3. The exponents of the correlation functions in both Luttinger and Luther-Emery liquids that decay with power laws can be characterized by a single parameter $K_\rho \geq 0$.[31,32] The nonoscillatory part of singlet pair correlation function decays as

$$\langle b^\dagger(r)b(0)\rangle \propto r^{-\lambda}, \tag{9}$$

where $b(r) = \frac{1}{\sqrt{2}}(c_{r\uparrow}c_{r+1\downarrow} - c_{r\downarrow}c_{r+1\uparrow})$. For Luttinger liquids $\lambda_L = 1 + K_\rho^{-1}$ while Luther-Emery liquids have $\lambda_{LE} = K_\rho^{-1}$.

In Fig. 3, $b(k)$ diverges logarithmically with system size as $k \to 0$ in our trial wave function, which represents the strongest divergence possible in a Luttinger-liquid state. However, the true ground state in this region apparently exhibits a much stronger cusp.[19]

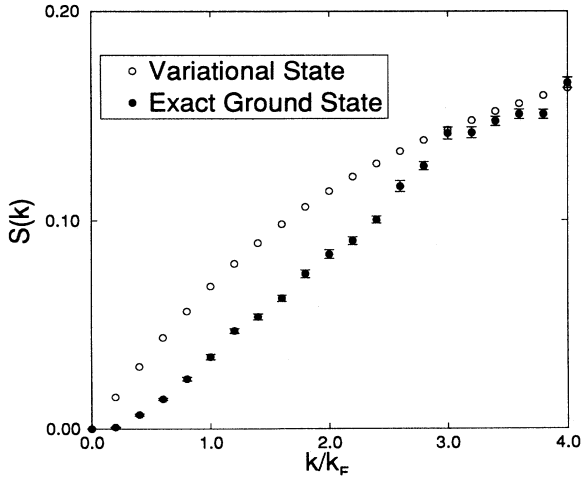

FIG. 2. The spin-spin correlation function for $J/t = 2.8$ and density $n = \frac{1}{6}$. The optimized variational wave function has linear behavior at small wave vectors while the exact spin correlation turns on quadratically in k. The system contains 20 electrons on a 120-site lattice.

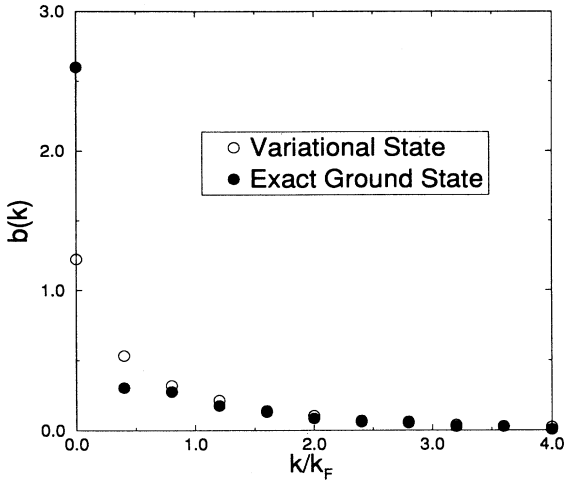

FIG. 3. The singlet pair correlation function at $J/t = 2.8$ and density $n = \frac{1}{6}$. The $k = 0$ cusp is greatly enhanced in the exact ground state. The system contains ten electrons on 60 sites.

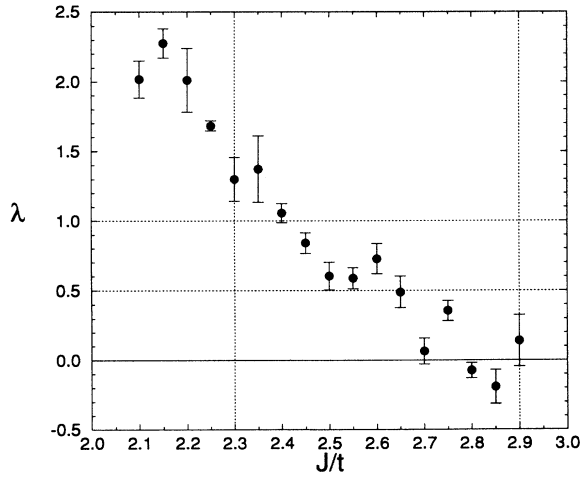

FIG. 4. The scaling of the exponent of the $k = 0$ superconducting cusp with interaction strength at density $n = \frac{1}{6}$. The transition from Luttinger to Luther-Emery-liquid states occurs at $J/t \approx 2.3$ and the system phase separates at $J/t \approx 2.9$. Luttinger liquids require $\lambda \geq 1$, and noninteracting hard-core bosons have $\lambda = \frac{1}{2}$.

Using a finite-size scaling analysis of the divergence in $b(k \to 0)$ in the projected state, we can determine the value of this exponent λ.[25] A plot of λ showing the transition from Luttinger to Luther-Emery-liquid behavior at density $\delta = 1/6$ is shown in Fig. 4. In the Luttinger regime, λ is bound from below by 1, but this bound is clearly violated as the Luther-Emery state is entered. A continuous variation of λ with J as found in these data would imply a discontinuous jump in K_ρ.

It is interesting to note that noninteracting hard-core bosons have $\lambda = 1/2$, so our singlet pairs have residual repulsive interactions for $J \lesssim 2.65$ in the Luther-Emery state, while at higher J the hard-core nature of the pairs competes with an effective attractive interaction.[33] The attraction from the Heisenberg term in (1) in this regime is strong enough to bind singlet pairs but still insufficient to cause macroscopic phase separation.

Chen and Lee proposed a variational state for this region by Gutzwiller projecting a sea of noninteracting bound singlet pairs.[20] Their wave function corresponds to a $K_\rho = \infty$ Luther-Emery state, the critical point of the verge of phase separation which exhibits a macroscopic superfluid density. Their calculations of the boundaries of the spin-gap regime agree remarkably well with ours except at the boundary to phase separation, which they find occurs at higher J/t. One may speculate that a potentially more accurate trial state could be generated by correlating the pairs with a Jastrow factor similar to (2). This state would exhibit generalized Luther-Emery behavior with arbitrary K_ρ.

In summary, we have investigated the ground-state properties of the t-J model in one dimension using a numerical technique to project the exact ground state from a variational Luttinger-liquid trial state. We find the model has a surprisingly rich phase diagram. At lower interaction strengths the variational wave function accurately describes the Luttinger-liquid phase, and at very large J/t the model phase separates. However, one finds these phases are separated at low density by a Luther-Emery quantum dimer liquid phase with short-range spin correlations and enhanced superconducting correlations.

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