Two-dimensional t-J model at low electron density

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The phase diagram of the two-dimensional t-J model is determined accurately at low electron density by a combination of analytic and numerical techniques. The ground state exhibits three phases in the limit of zero-electron density: an unpaired state at small J/t, a gas of s-wave pairs for $2 < J/t \lesssim 3.4367$, and a phase-separated state at larger interaction strengths. Bound states of larger clusters are never realized, and the instabilities present at small densities are discussed.

Models of strongly correlated electrons have received renewed attention since the discovery of the cuprate superconductors.[1] However, a reliable method of calculating ground-state properties of such models on dense large-size systems has not yet been demonstrated.

In this paper, we concentrate on the low *electron* density limit of the two-dimensional t-J model, one of the simplest models with strong correlation.[2–5] This limit appears far from the small *hole* densities thought to be applicable to cuprate superconductivity, but it is important to calculate the entire phase diagram of the model. A complete description of the low electron density limit, where much can be calculated analytically, yields a solid basis from which to move into the potentially more interesting regions of the model. Additionally, we introduce and test a numerical technique that we expect will prove to be a powerful tool for investigating strongly correlated models at higher electron densities.

The t-J Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + J \sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right) \tag{1}$$

acts only on the constrained Hilbert space with no doubly occupied sites. The operator $c^{\dagger}_{i\sigma}$ creates an electron of spin σ on site i, $\mathbf{S}_i$ is the spin operator, and $n_i = \sum_{\sigma} c^{\dagger}_{i\sigma} c_{i\sigma}$. The sum over $\langle ij \rangle$ enumerates nearest-neighbor bonds of a square lattice.

As $J/t \to 0$, the electrons separate to avoid interactions in the limit of zero density, and the ground-state energy per particle is the kinetic energy of free electrons, $\mathcal{E}_{N=1} = -4t$. Assuming a macroscopic number of electrons, the system phase separates completely in the large interaction strength limit, and the energy per particle, $\mathcal{E}_{N=\infty} = -1.169\,34J \pm 0.000\,03J$, comes purely from the interaction term in (1). This value is the result of the most accurate calculation of the ground-state energy of the Heisenberg model[6] shifted by $-\frac{1}{4}J$ per bond.

For intermediate interaction strengths, the situation becomes more complicated. It is well known that for $J/t > 2$, pairs of electrons bind into an s-wave state.[3,4] However, previous work only cursorily examined the transition from this pairing phase to the completely phase-separated state at large J/t.

This paper presents a thorough calculation of the phase diagram of the two-dimensional t-J model at zero-electron density. We calculate the energy per particle of all potential intermediate phases as a function of J/t. We show that no intervening phase is stabilized between the gas of s-wave pairs and the completely phase-separated state, and we determine the phase boundaries accurately. Finally, we discuss possible instabilities at low densities.

The energy of a bound electron pair may be found analytically, and we give the exact solutions below. In the limit of large J/t, a pair binds into a singlet dimer with an energy per particle of $\mathcal{E}_{N=2} = -\frac{1}{2}J$. Since the chemical potential of three bound electrons is the same in the strong interaction limit, we dismiss three-particle bound states as a viable intermediate phase.

The next competitive intervening phase to consider is a gas of bound quartets. Four electrons bind into a square configuration with an energy $\mathcal{E}_{N=4} = -\frac{3}{4}J$ per particle in the large J/t limit. Since this value is significantly lower than the pair chemical potential, quartets warrant careful scrutiny as a potential ground-state phase. We use a Green's function Monte Carlo method to solve the four-body problem on finite lattices and extrapolate to infinite system size. Close to the critical J/t for four electrons to bind, the weakly bound quartets are very extended objects. An accurate calculation of this critical interaction strength on the infinite lattice requires precise ground-state energies of four electrons on very large lattices. With the computational method described below, we can calculate ground-state properties on lattices with dimensions as large as 20×20. The results enable us to determine that bound quartets are never energetically stabilized in a macroscopic system.

The paper is organized as follows: The solutions of two and four particles on the infinite lattice are outlined. We then calculate and discuss the low-density phase diagram.

The equations of motion of two electrons yield two bound states for sufficiently large interaction strengths, one with s-wave symmetry and one with $d_{x^2-y^2}$-wave symmetry.[4,7–9] The analysis is simplified by defining the reduced s-wave pair binding energy $\delta_s = (-8t - E_s)/8 \geq 0$, where E_s is the total energy of the s-wave pair. The reduced d-wave pair binding energy δ_d is defined similarly.

On the infinite lattice, the s-wave solution satisfies

$$\frac{1}{J}=\frac{1+\delta_s}{2}\left[1-\frac{\pi}{2}\Big/K\left(\frac{1}{1+\delta_s}\right)\right], \tag{2}$$

where $K(k)$ is the complete elliptic integral of the first kind.[4] From now on, we express all energy scales in units of t. This expression may be expanded close to the critical J for pairs to bind. To order δ_s, we find

$$\frac{1}{J}\approx\frac{1}{J_c^s}+\frac{\pi}{2}\frac{1}{\ln(\delta_s/8)}+\frac{1}{2}\delta_s+\frac{\pi}{4}\frac{\delta_s}{\ln(\delta_s/8)}+\cdots, \tag{3}$$

where $J_c^s=2$ is the critical interaction strength to bind s-wave pairs. An expansion may also be made for large binding energy.[4,8]

After a similar analysis to that given in Ref. 4, the large-lattice limit of the d-wave solution reduces to

$$\frac{1}{J}=\frac{2+\delta_d}{\pi}E\left(\frac{\sqrt{1+\delta_d}}{1+\delta_d/2}\right)-\frac{1+\delta_d}{2}, \tag{4}$$

where $E(k)$ is the complete elliptic integral of the second kind. An expansion for small binding energy yields

$$\frac{1}{J}\approx\frac{1}{J_c^d}-\frac{\pi-2}{2\pi}\delta_d-\frac{\delta_d^2\ln\delta_d}{4\pi}+\frac{6\ln 2-1}{8\pi}\delta_d^2+\cdots, \tag{5}$$

where the critical interaction strength for d-wave pairing is $J_c^d=2\pi/(4-\pi)\approx 7.32$.

We solve the four-electron problem with a version of Green's function Monte Carlo (GFMC).[9–12] We project a trial state onto the ground state by operating on it repeatedly with the Hamiltonian. This generates a series of increasingly accurate approximants to the ground state labeled by integers $|p\rangle=H^p|\Psi\rangle$.

It is useful to expand the trial state in terms of the exact eigenstates:

$$|\Psi\rangle=a_0|\Psi_0\rangle+a_1|\Psi_1\rangle+a_2|\Psi_2\rangle+\cdots, \tag{6}$$

where $|\Psi_0\rangle$ is the ground state, $|\Psi_1\rangle$ is the first excited state, etc., and the a_i's are the expansion coefficients. Rewriting the projected states in this way, we see

$$|p\rangle\propto|\Psi_0\rangle+\frac{a_1}{a_0}\left(\frac{E_1}{E_0}\right)^p|\Psi_1\rangle+\frac{a_2}{a_0}\left(\frac{E_2}{E_0}\right)^p|\Psi_2\rangle+\cdots, \tag{7}$$

where E_i is the energy of the ith eigenstate. Thus, $|p\rangle$ approaches the lowest eigenstate for large p provided $a_0\neq 0$ and $|E_{i>0}|<|E_0|$ for all excited state energies $E_{i>0}$, a condition satisfied by the t-J model for $J>0$.

Care is needed to choose a trial state having maximal overlap with the true ground state. We try to write a very general form for the trial state, but restrict it to be a spin singlet with zero total momentum. We use the Jastrow-pairing state:

$$|\Psi\rangle=\prod_{i<j}f(\mathbf{r}_i-\mathbf{r}_j)P_4\prod_{\mathbf{k}}(u_{\mathbf{k}}+v_{\mathbf{k}}c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger)|0\rangle, \tag{8}$$

where $c_{\mathbf{k}\sigma}^\dagger$ is the Fermion creation operator and P_4 projects the state onto the subspace with four particles.[13] We use mixed boundary conditions, since the GFMC converges faster with a closed shell. All boundary conditions extrapolate to the same value in the infinite system.

The Jastrow factor $f(\mathbf{r})$ correlates *all* pairs of particles, yielding a total-spin-singlet state. We satisfy the t-J model's hard-core constraint by requiring $f(\mathbf{r}=\mathbf{0})=0$.

The GFMC needs a positive-definite guiding function, which we take to be

$$\Psi^g=\prod_{i<j}f^g(\mathbf{r}_i-\mathbf{r}_j)\prod_{i',j'}s^g(\mathbf{r}_{i'\uparrow}-\mathbf{r}_{j'\downarrow}). \tag{9}$$

In general, $f^g(\mathbf{r})\neq f(\mathbf{r})$. Since it is not important to guide with a spin-singlet function, we use the additional spin-dependent Jastrow factor $s^g(\mathbf{r})$ in the guiding function. The primed indices enumerate electrons of one spin.

Auspicious choices of trial and guiding states can drastically reduce the statistical errors in the GFMC. We use much more general and potentially far superior states than previous work. Since the electrons on a given size lattice only occupy a finite number of locations $\mathbf{r}$, we let the factors in (8) and (9) vary independently at each distance or wave vector not related by symmetry. We apply all rotation and mirror symmetries to the Jastrow factors, but only the mirror symmetries about the axes and parity to the Fermion pairing fields $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. For example, the Fermion pairing fields may be any real linear combination of an s and $d_{x^2-y^2}$ pairing state, but time-reversal breaking and d_{xy} symmetries are excluded.

On a 20×20 lattice, each Jastrow factor has 400 parameters, as do the Fermion pairing fields. The symmetry restrictions reduce the 800 total parameters in each state to 172 independent parameters in the trial state and 128 in the guiding function. To optimize the parameters, we minimize the variance of the local energy.[14] For sufficiently large J/t, we find the spin-independent Jastrow factors in (8) and (9) bind the electrons in the optimized state, while the pairing fields $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ and the guiding function's spin-dependent Jastrow factor $s^g(\mathbf{r})$ provide the internal correlation of the bound quartet.

The statistical errors increase exponentially with increasing power p, so we use the GFMC output at small powers to extrapolate to infinite power. We assume that the expansion (6) can be approximated by a small number of terms, typically about five, and we fit the output to determine the coefficients a_i and energies E_i. We include enough terms in (6) to make the systematic error due to omitting terms smaller than the statistical errors.

Previous work[9,10] fit the GFMC output to

$$\frac{\langle p|H|p\rangle}{\langle p|p\rangle}=\frac{\langle\Psi|H^{2p+1}|\Psi\rangle}{\langle\Psi|H^{2p}|\Psi\rangle} \tag{10}$$

$$=\sum_i|a_i|^2E_i^{2p+1}\Big/\sum_i|a_i|^2E_i^{2p}\ \stackrel{p\to\infty}{\longrightarrow}\ E_0. \tag{11}$$

Figure 1 shows a nicely converged example in this form. While this function has the advantage of converging to the ground-state energy for large p, it is quite difficult to fit (11) with more than two terms in (6). We instead fit the simpler function

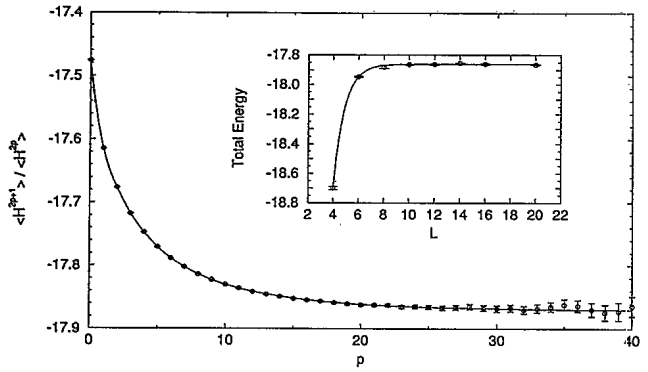

FIG. 1. Plot of the GFMC output in the form of Eq. (10) for four electrons on a 20×20 lattice with $J/t = 5.5$. The data converge to the total ground-state energy at large power p. The solid line is the fit to (11) taking five terms in (6). The inset shows the scaling of the total ground-state energy with linear system size L. The fit to (13) is used to extrapolate to the infinite system.

$$\frac{\langle\Psi|H^p|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_i |a_i|^2 E_i^p \overset{p\to\infty}{\longrightarrow} |a_0|^2 E_0^p \qquad (12)$$

to determine all the coefficients a_i and energies E_i.

For each value of J/t, we calculate the ground-state energy on square lattices of dimensions $L \times L$, where L ranges from $L = 4$ to $L = 20$. We expect the energy of a bound state to converge exponentially with linear system size. To determine the infinite-lattice ground-state energy $E(L = \infty)$, we fit the finite results to

$$E(L) = E(L = \infty) - D\exp(-L/\xi)\ , \qquad (13)$$

where $E(L)$ is the ground-state energy on an $L \times L$ lattice, and $D > 0$ and $\xi > 0$ are parameters. The inset in Fig. 1 shows a sample extrapolation with system size.

The energies of each phase are shown in Fig. 2. The two-particle bound-state energies plotted are the exact expressions obtained by solving the integral equations (2) and (4). The s-wave pair binds with a weak logarithm beyond the critical interaction strength $J_c^s = 2$, while the d-wave binding energy turns on with a healthy linear term for $J > J_c^d \approx 7.32$. The four-particle energies are extrapolated to infinite system size. Below the critical J to bind quartets, the energies per particle of the four-electron system are the same as that of the s-wave pair.

Only three of the phases considered are realized as ground states. For $J \leq 2$, the electrons are free, minimizing their kinetic energy. At larger interaction strengths, they bind into s-wave pairs, and finally the system undergoes macroscopic phase-separation to form a Heisenberg cluster. The transition to complete phase separation occurs at $J_c^{ps} = 3.4367 \pm 0.0001$, which is determined by equating the phase-separated energy with the solution of (2). The statistical error of the transition point is due to the uncertainty in the best estimate of the ground-state energy of the Heisenberg model.[6]

It is obvious from Fig. 2 that four-particle bound states are never stabilized in a macroscopic system. To determine the critical interaction J_c^q for two pairs of electrons to bind into a four-particle state, we fit the quartet binding energies close to the transition to the form

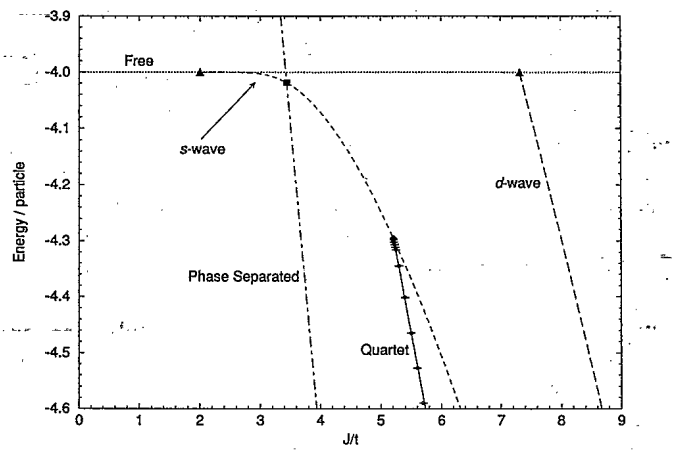

FIG. 2. Energy per particle for each phase at zero-electron density. The horizontal dotted line is the kinetic energy of free electrons, and the dot-dashed line is the potential energy of the macroscopically phase-separated system. The short-dashed and long-dashed lines are the energies of s-wave and d-wave two-particle bound states, respectively. Their intersections with the free-electron energy are marked with triangles, and the intersection of the s-wave pair energy with the phase-separated energy is marked with the square. The circles with error bars are the four-particle energies, and the solid line is the best fit of the quartet binding energies to (14). The fit intersects the s-wave energy at the diamond.

$$\frac{1}{J} = \frac{1}{J_c^q} + \frac{A}{\ln\delta_4 + B} + C\delta_4\ , \qquad (14)$$

where $A \geq 0$, B, and C are parameters. The binding energy is given by $\delta_4 = -(E_{N=4} - 2E_s) \geq 0$, where $E_{N=4}$ and E_s are the total infinite-lattice ground-state energies of the four-particle and s-wave pair states, respectively. Since we have no analytic form for the scaling of the quartet energies, we generalize the first three terms in the expansion of the s-wave pair binding energy (3) to obtain (14). This form also includes the first two terms of the expansion of the d-wave pair binding energy (5).

The transition for pairs to bind into quartets occurs at $J_c^q = 5.21 \pm 0.03$. The statistical error is largely due to the singular nature of the fitting function (14). It is clear that the quartet phase is never energetically favorable to the macroscopically phase-separated state. The fit to (14) is shown as the solid line in Fig. 2. Both the phase-separation point, J_c^{ps}, and the quartet binding point were calculated incorrectly in previously published work.[3,4]

Because the four-body energy per particle is higher than that of the phase-separated state, we see no need to consider gases of larger clusters as potential ground states. In the limit of large particle number N, the energy per electron of a finite bound droplet scales as

$$\mathcal{E}_N \approx \mathcal{E}_{N=\infty} + \alpha/\sqrt{N} + \cdots, \qquad (15)$$

where $\mathcal{E}_{N=\infty}$ is the bulk energy per particle of the phase-separated state and $\alpha > 0$ is the surface correction. Since the surface correction is positive, the energies of large clusters approach the phase-separated energy monotonically from *above* with increasing droplet size, and $\mathcal{E}_N > \mathcal{E}_{N=\infty}$ for sufficiently large N. Clearly this inequality is violated for $N = 2$, but we have shown it holds for $N = 4$. Assuming the energy per particle of clusters is a reasonably smooth function of cluster size, the phase-separated state will have lower energy per electron than all droplets with four or more particles. Thus, the zero-electron-density phase diagram consists only of the three phases described above.

At low but nonzero electron densities, both the phase-separated and s-wave pair states, which have single-particle excitation gaps, remain robust. However, the phase of free electrons at $J \leq 2$ is unstable to higher-angular-momentum pairings similar to the Kohn-Luttinger effect in three dimensions.[15,16] Using expressions (20) and (21) in Ref. 15, we find the phase diagram shown in Fig. 3, which differs substantially from the phase diagram in that reference. As the electron density increases from zero, the phase-separated and s-wave pairing states persist, but the free-electron phase is unstable to p-wave pairing at small J and $d_{x^2-y^2}$ pairing at larger J. The energy gaps in these higher-angular-momentum pairing states increase from zero with increasing density, but remain extremely small at the low densities where the effect is valid. For example, at electron density $n = 0.1$, all p and d-wave energy gaps are less than $10^{-7}t$.

In summary, we have calculated the complete phase diagram of the two-dimensional t-J model in the limit of low electron density and corrected errors in previously published work. The phase-separated state at large J evaporates into a gas of s-wave pairs as the interaction strength is reduced—gases of larger finite clusters are never stabilized. The s-wave pairs unbind as J is reduced further, but the resulting Fermi liquid is unstable first to d-wave pairing and finally to p-wave pairing.

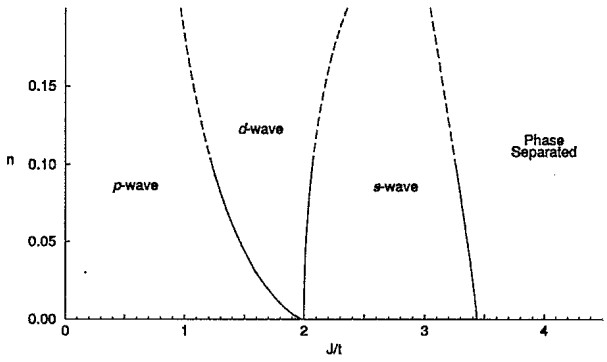

FIG. 3. Phase diagram for low electron density. The phase-separation boundary is estimated from the two-body solution on finite systems, and the other lines are calculated from expressions in Ref. 15. All phase boundaries become less accurate with increasing electron density per site n.

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