EXACT ANALYTIC APPROACHES TO THE TWO-DIMENSIONAL t-J MODEL AT LOW ELECTRON DENSITY

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ABSTRACT

The phase diagram of the two-dimensional t-J model in the limit of infinitesimal electron density is determined exactly with analytic approaches. Numerical work is only required to show other potential ground states are never stabilized. Significant differences with previous work on the model are found. The ground state exhibits pairing for all interaction strengths insufficient to cause phase separation. The pairing is p-wave for small interaction strengths, $d_{x^2-y^2}$ for intermediate J/t, and s-wave for larger J/t.

Since the discovery of the cuprate superconductors, models of strongly correlated electrons have received renewed attention.[1] In this paper, we consider the low *electron* density limit of the two-dimensional t-J model, one of the simplest models with strong correlation.[2,3,4,5,6] This limit appears far from the small *hole* density 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 yields a solid basis from which to move into the potentially more interesting regions of the model. Since we find significant discrepancies with previous work, a reexamination of this limit of the model was long overdue.

The t-J Hamiltonian can be written as

$$H = -t \sum_{\langle i,j\rangle,\sigma} \left(a^\dagger_{i\sigma} a_{j\sigma} + a^\dagger_{j\sigma} a_{i\sigma} \right) + J \sum_{\langle i,j\rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right). \tag{1}$$

Here, $\mathbf{S}_i$ is the spin operator, $n_i = \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma}$, and $a^\dagger_{i\sigma} = (1 - n_{i-\sigma}) c^\dagger_{i\sigma}$ creates an electron of spin σ on site i while obeying the no double occupancy constraint. The sum over $\langle i,j\rangle$ enumerates nearest-neighbor bonds of a square lattice.

In the large J/t limit, the model phase separates, and the ground state energy comes purely from the interaction term in (1). This energy is simply the ground state energy of the Heisenberg model shifted by $-\frac{1}{4}J$ per bond.[2] Prior to phase separation, the model is susceptible to two sources of pairing instabilities. We first solve the two-body problem on the infinite lattice and show s-wave pairs are stabilized for $2 < J/t < 3.4367$ in the limit of zero density. We then discuss the additional instabilities present at small non-zero electron densities.

The ground state of two electrons in the t-J model may be solved analytically, yielding two bound states with s-wave and $d_{x^2-y^2}$-wave symmetry for sufficiently large

J/t.[4,6,7] The analysis is simplified by relaxing the no-double occupancy constraint of (1) and adding an on-site repulsion. The generalized Hamiltonian is given by

$$H' = -t \sum_{\langle i,j\rangle,\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \right) + J \sum_{\langle i,j\rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{2}$$

and we recover the original t-J Hamiltonian by taking the $U \to \infty$ limit. Since the nearest-neighbor interaction term is attractive only between electrons in a spin-singlet state, we may ignore triplet solutions. If we write the ground state wave function with zero total momentum in terms of the relative separation between the particles:

$$|\Psi\rangle = \sum_{\mathbf{r}_1,\mathbf{r}_2} \Psi(\mathbf{r}_1 - \mathbf{r}_2) c^\dagger_{\mathbf{r}_1\uparrow} c^\dagger_{\mathbf{r}_2\downarrow} |0\rangle. \tag{3}$$

the Schrödinger equation in momentum space becomes

$$(E + 2\varepsilon(\mathbf{q}))\,\Phi(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{k}} (U - J\varepsilon(\mathbf{q} - \mathbf{k}))\,\Phi(\mathbf{k}), \tag{4}$$

where we have substituted $\varepsilon(\mathbf{q}) = 2(\cos q_x + \cos q_y)$ as the single particle dispersion, and E is the total energy of the two electron system. From now on, we express all energy scales in units of t. Transformed back into real space, we find that (4) couples the on-site and nearest-neighbor amplitudes of Ψ by

$$\begin{pmatrix} UI_0 & -2JI_x & -2JI_y \\ UI_x & -2JI_{xx} & -2JI_{xy} \\ UI_y & -2JI_{xy} & -2JI_{yy} \end{pmatrix} \begin{pmatrix} \Psi(\mathbf{0}) \\ \Psi(\hat{\mathbf{x}}) \\ \Psi(\hat{\mathbf{y}}) \end{pmatrix} = \begin{pmatrix} \Psi(\mathbf{0}) \\ \Psi(\hat{\mathbf{x}}) \\ \Psi(\hat{\mathbf{y}}) \end{pmatrix} \tag{5}$$

where we have introduced the notation

$$I_0 = \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{E + 2\varepsilon(\mathbf{q})}, \qquad I_x = \frac{1}{N} \sum_{\mathbf{q}} \frac{\cos q_x}{E + 2\varepsilon(\mathbf{q})},$$
$$I_{xx} = \frac{1}{N} \sum_{\mathbf{q}} \frac{\cos^2 q_x}{E + 2\varepsilon(\mathbf{q})}, \qquad I_{xy} = \frac{1}{N} \sum_{\mathbf{q}} \frac{\cos q_x \cos q_y}{E + 2\varepsilon(\mathbf{q})}, \tag{6}$$

and $I_y = I_x$ and $I_{yy} = I_{xx}$.

Equation (5) has two solutions: A $d_{x^2-y^2}$-wave state with $\Psi(\hat{\mathbf{x}}) = -\Psi(\hat{\mathbf{y}})$ where

$$\frac{1}{J^{(d)}} = 2\,(I_{xy} - I_{xx}) \tag{7}$$

and an s-wave state with $\Psi(\hat{\mathbf{x}}) = \Psi(\hat{\mathbf{y}})$ where

$$\frac{1}{J^{(s)}} = \frac{4UI_x^2}{UI_0 - 1} - 2\,(I_{xx} + I_{xy}). \tag{8}$$

The s-wave solution may be simplified with the relations

$$I_{xx} + I_{xy} = -\frac{E}{4} I_x, \qquad I_x = \frac{1}{8} - \frac{E}{8} I_0, \tag{9}$$

and we find, in the $U \to \infty$ limit, the s-wave solution becomes

$$\frac{16}{J^{(s)}} = \frac{1}{I_0} - E. \tag{10}$$

In the large lattice limit, I_0 can be written in terms of $\boldsymbol{K}(k)$, the complete elliptic integral of the first kind, by rotating the obvious axes of integration[8]

$$\begin{aligned} I_0 &= \frac{1}{\pi^2} \int_0^\pi dx \int_0^\pi dy \frac{1}{E + 4\cos x + 4\cos y} \\ &= \frac{1}{\pi^2} \int_0^\pi dx' \int_0^\pi dy' \frac{1}{E + 8\cos x' \cos y'} \\ &= \frac{1}{E} \frac{2}{\pi} \boldsymbol{K}(8/E), \end{aligned} \tag{11}$$

so the critical interaction strength for two free electrons, with total energy $E_0 = -8t$, to bind into an s-wave state is $J_c^{(s)} = 2$.

Similarly, the large lattice limit of the d-wave solution (7) reduces to

$$\begin{aligned} \frac{1}{J^{(d)}} &= \frac{1}{\pi^2} \int_0^\pi dx \int_0^\pi dy \frac{-(\cos x - \cos y)^2}{E + 4\cos x + 4\cos y} \\ &= \frac{4}{\pi^2} \int_0^\pi dx' \int_0^\pi dy' \frac{-\sin^2 x' \sin^2 y'}{E + 8\cos x' \cos y'} \\ &= \frac{E}{8\pi} \left[\left(1 - (8/E)^2\right) \boldsymbol{K}(8/E) - 2\boldsymbol{E}(8/E) \right] + \frac{E}{16} \\ &= \frac{8 - E}{8\pi} \boldsymbol{E}\left(\frac{2\sqrt{-8E}}{8 - E} \right) + \frac{E}{16}, \end{aligned} \tag{12}$$

where $\boldsymbol{E}(k)$ is the complete elliptic integral of the second kind. The critical interaction strength for d-wave pairing is $J_c^{(d)} = 2\pi/(4 - \pi) \approx 7.32$. The s-wave state always has lower energy than the d-wave, and a gas of s-wave pairs phase separates at $J_c^{(ps)} = 3.4367$.[9] This point was calculated incorrectly in previous work.[3,4]

To calculate the complete phase diagram, we must check the stability of larger clusters of electrons on the otherwise empty lattice. In the infinite J/t limit, the smallest cluster with lower energy per particle than the s-wave pair is four electrons in a square configuration. For arbitrary interaction strengths, this problem cannot be solved analytically, so we have calculated the exact ground state energy of four electrons on the infinite lattice with a newly developed Green's Function Monte Carlo (GFMC) technique for lattice Fermions.[9,10]

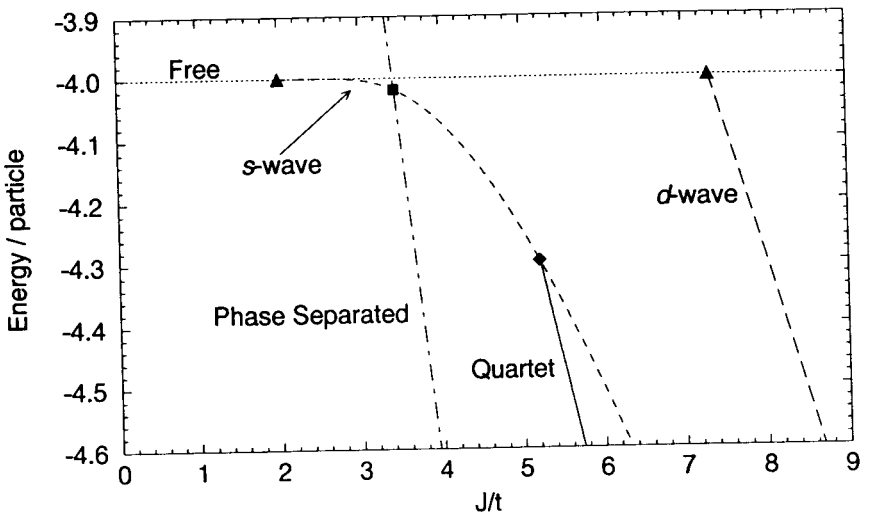

Figure 1: Energy per particle in units of t for each phase at zero electron density. The horizontal dotted line is the free electron kinetic energy, and the dot-dashed line is the potential energy of the phase-separated system. The short-dashed and long-dashed lines are the energies of s-wave and d-wave 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 solid line is the energy of the four-particle bound state determined numerically in Ref. 9. It intersects the s-wave energy at the diamond.

The energy of each phase is plotted in Fig. 1. The pair ground state energies are calculated from (10) and (12), while the quartet energies are the GFMC results. The zero-density ground state consists of free electrons for $J/t \leq 2$, s-wave pairs for intermediate interaction strengths, and a phase separated state for $J/t > 3.4367$. Quartets and d-wave pairs are never stabilized. We cannot exclude the possibility that larger clusters are stabilized between the s-wave and phase separated ground states, but such a scenario is highly unlikely. The energy per electron of very large clusters must converge to the phase-separated energy as a function of cluster size from *above* due to surface effects. Since the energy per particle of the four-electron bound state already exceeds that of the phase separated state, no larger clusters can be stabilized as ground states if the energy is a reasonably smooth function of cluster size.

At small but non-zero electron densities, the model has additional instabilities due to higher-angular-momentum scattering across the Fermi surface similar to the Kohn-Luttinger (KL) effect. Kagan and Rice[11] studied these pairings by solving the

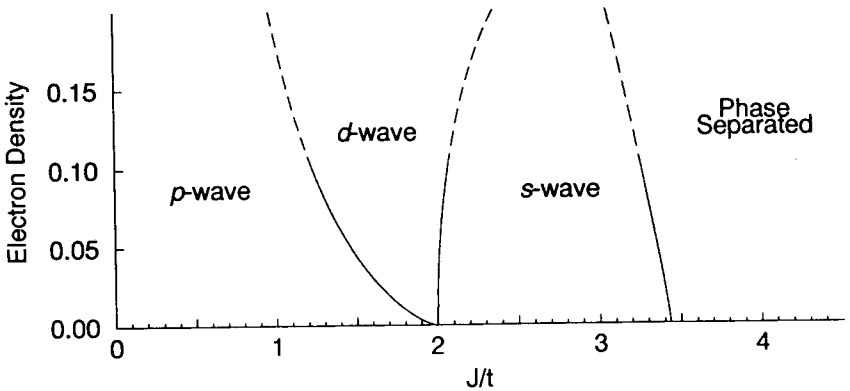

Figure 2: Phase diagram for low electron density. The phase-separation boundary is calculated from the two-body solution on finite systems, and the other lines are calculated from expressions in Ref. 11. All phase boundaries become less accurate with increasing electron density per site.

Cooper problem in the t-J model in the T-matrix approximation, which is accurate in the low density limit. Using expressions from Ref. 11, we calculate the low-density phase diagram shown in Fig. 2, which differs substantially from the phase diagram in that Reference. The KL p-wave instability exists for all $J/t < 2$, while there is a $d_{x^2-y^2}$ instability for all $J > 0$. The ground state at each point in the phase diagram simply corresponds to the strongest instability.

The essence of the KL effect stems from the fact that a short-ranged *repulsive* interaction in real space can be effectively *attractive* in non-zero angular momentum channels in the presence of a Fermionic background.[12] The strength of these instabilities scales with the size of the Fermi surface, and thus with the density, but remains extremely weak at the densities where the T-matrix approach is valid. Even at the arguably high electron density of $n = 0.1$, the energy of this effect is many orders of magnitude smaller than the other energy scales in the problem. The single-particle energy gaps of each phase at this density are plotted in Fig. 3. In a plot of this type, the ground state is given by the phase with the largest gap.

In summary, we have calculated the phase diagram of the two-dimensional t-J model in the limit of low electron density exactly. The electrons are paired for all interaction strengths insufficient to cause phase separation. For $J/t > 2$, the ground state consists of strongly bound s-wave pairs, while for smaller J/t, there are extremely weak instabilities to p-wave and d-wave pairing.

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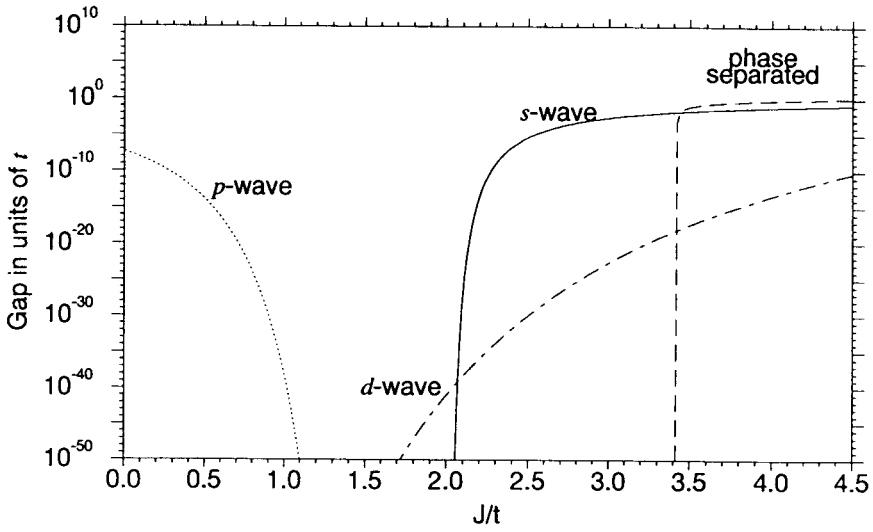

Figure 3: Single particle energy gaps at electron density $n = 0.1$. The ground state for a given J/t is the phase with the largest gap.

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