Dilute gas of electron pairs in the t-J model

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(Received 3 December 1990; revised manuscript received 1 April 1991)

The bound state of electron pairs in the t-J model is investigated. It is shown that for $2t < J < 3.828t$ the hole-rich phase is a low-density superfluid of electron pairs.

Since the discovery of high-temperature superconductors,[1] many of the theoretical studies have focused on the motion of holes in antiferromagnets. Of the various models proposed, the simplest and most widely studied one is the t-J model.[2] It starts from the assumption that the parent compounds are well represented by the antiferromagnetic Heisenberg model with localized electrons of spin-$\frac{1}{2}$ occupying a square lattice and coupled by an exchange integral J. Doping is assumed to remove electrons, thereby producing "holes" which are mobile because neighboring electrons can hop to the hole site with amplitude t. Recently, Emery, Kivelson, and Lin[3] have shown that, for the t-J model, dilute holes in an antiferromagnet are unstable against phase separation into a hole-rich and a no-hole phase. They obtained a critical value J_c such that when the spin-exchange interaction J exceeds J_c, the hole-rich phase has no electrons. It was proposed that for J slightly less than J_c the hole-rich phase is a low density superfluid of electron pairs. The purpose of this paper is to present a more detailed study of this problem.

Let us start by showing the condition for a two-particle bound state explicitly. To simplify the mathematics, we add a Hubbard interaction $Un_{i\uparrow}n_{i\downarrow}$ to the t-J model and relax the constraint that there be no doubly occupied sites. Hence the model Hamiltonian is given by

$$H = -t \sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^{\dagger}c_{j\sigma} + J\sum_{\langle i,j\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j - \tfrac{1}{4}n_i n_j) + U\sum_i n_{i\uparrow}n_{i\downarrow} \ , \tag{1}$$

where $c_{i\sigma}^{\dagger}$ creates an electron of spin σ on site i and n_i, $\mathbf{S}_i$ are the electron-number and spin operators, respectively. $\langle i,j\rangle$ denotes the nearest-neighbor pairs. By setting $U=\infty$ we recover the t-J model, which is the first two terms in Eq. (1), subject to the constraint that there be no doubly occupied sites. It is clear that there is an attractive potential $(-J)$ between electrons in singlet states on neighboring sites, so for sufficiently large values of J a bound state of electrons should exist. Our first step is thus to determine the critical value of J_{2c} such that for $J \geq J_{2c}$, two otherwise "free electrons" can form a two-particle bound state.

For a system consisting of two electrons the wave function can be written in the form

$$\Psi = \sum_{i_1,i_2} \Phi(i_1,i_2) c_{i_1\uparrow}^{\dagger} c_{i_2\downarrow}^{\dagger} |0\rangle \ , \tag{2}$$

where $|0\rangle$ denotes the vacuum state. It is well known that for a two-body problem the ground state is a singlet, $\Phi(i_1,i_2)=\Phi(i_2,i_1)$, and the equation of motion is

$$E\Phi(i_1,i_2) = \sum_j [t_{i_1 j}\Phi(j,i_2) + t_{i_2 j}\Phi(i_1,j)] + [U\delta_{i_1,i_2} - J_{i_1,i_2}]\Phi(i_1,i_2) \ , \tag{3}$$

where $t_{ij}(J_{ij}) = -t(J)$ if (i,j) are nearest-neighbor pairs, and zero otherwise. For a system with periodic boundary conditions, we can use Fourier transforms to rewrite Eq. (3) as

$$E\Phi(\mathbf{k}_1,\mathbf{k}_2) = [t(\mathbf{k}_1)+t(\mathbf{k}_2)]\Phi(\mathbf{k}_1,\mathbf{k}_2) + \frac{U}{N}\sum_{\mathbf{k}}\Phi(\mathbf{k}_1+\mathbf{k},\mathbf{k}_2-\mathbf{k}) - \frac{1}{N}\sum_{\mathbf{k}} J(\mathbf{k})\Phi(\mathbf{k}_1-\mathbf{k},\mathbf{k}_2+\mathbf{k}) \ , \tag{4}$$

where

$$\Phi(\mathbf{k}_1,\mathbf{k}_2) = \frac{1}{N}\sum_{i_1,i_2}\Phi(i_1,i_2)e^{-i\mathbf{k}_1\cdot\mathbf{r}_{i_1} - i\mathbf{k}_2\cdot\mathbf{r}_{i_2}} \ , \tag{5}$$

$$t(\mathbf{k}) = \frac{1}{N}\sum_{i,j} t_{ij} e^{-\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} = -2t(\cos k_x + \cos k_y) \ , \tag{6}$$

$$J(\mathbf{k}) = 2J(\cos k_x + \cos k_y) \ . \tag{7}$$

Since the system is translationally invariant, the total momentum can be used to specify its eigenstates. Define $\mathbf{Q}=\mathbf{k}_1+\mathbf{k}_2$, $\mathbf{q}=\frac{1}{2}(\mathbf{k}_1-\mathbf{k}_2)$, and $\Phi(\mathbf{k}_1,\mathbf{k}_2)=\Phi_{\mathbf{Q}}(\mathbf{q})$. We then obtain

$$\Phi_{\mathbf{Q}}(\mathbf{q}) = \frac{\frac{U}{N}\sum_{\mathbf{k}}\Phi_{\mathbf{Q}}(\mathbf{k}) - \frac{1}{N}\sum_{\mathbf{k}} J(\mathbf{q}-\mathbf{k})\Phi_{\mathbf{Q}}(\mathbf{k})}{E - t\left[\frac{\mathbf{Q}}{2}+\mathbf{q}\right] - t\left[\frac{\mathbf{Q}}{2}-\mathbf{q}\right]} \ . \tag{8}$$

The interaction is separable and the integral equation, Eq. (4), may be transferred into a set of 3×3 algebraic equations:

$$D \equiv \frac{U}{N}\sum_{\mathbf{q}}\Phi_{\mathbf{Q}}(\mathbf{q}) = UI_0 D + UI_x - 2JC_x + UI_y - 2JC_y \ , \tag{9}$$

$$C_x \equiv \frac{1}{N}\sum_{\mathbf{q}} \cos q_x \Phi_{\mathbf{Q}}(\mathbf{q}) = I_x D + I_{xx} - 2JC_x + I_{xy} - 2JC_y , \quad (10)$$

$$C_y \equiv \frac{1}{N}\sum_{\mathbf{q}} \cos q_y \Phi_{\mathbf{Q}}(\mathbf{q}) = I_y D + I_{xy} - 2JC_x + I_{yy} - 2JC_y , \quad (11)$$

where

$$\varepsilon_{\mathbf{Q}}(\mathbf{q}) = t\left[\frac{\mathbf{Q}}{2}+\mathbf{q}\right] + t\left[\frac{\mathbf{Q}}{2}-\mathbf{q}\right] ,$$

$$I_0 \equiv \frac{1}{N}\sum_{\mathbf{q}} \frac{1}{E-\varepsilon_{\mathbf{Q}}(\mathbf{q})} ,$$

$$I_x \equiv \frac{1}{N}\sum_{\mathbf{q}} \frac{\cos q_x}{E-\varepsilon_{\mathbf{Q}}(\mathbf{q})} , \quad (12)$$

$$I_{xx} \equiv \frac{1}{N}\sum_{\mathbf{q}} \frac{\cos^2 q_x}{E-\varepsilon_{\mathbf{Q}}(\mathbf{q})} ,$$

$$I_{xy} \equiv \frac{1}{N}\sum_{\mathbf{q}} \frac{\cos q_x \cos q_y}{E-\varepsilon_{\mathbf{Q}}(\mathbf{q})} ,$$

and $I_y = I_{x\to y}$, $I_{yy} = I_{xx\to yy}$. For the s-wave solution (for which $\mathbf{Q}=\mathbf{0}$) we have $I_y = I_x$, $I_{xx} = I_{yy}$, and $C_x = C_y$ and the condition for having a solution is

$$-2J = \frac{1-UI_0}{2UI_x^2 + (I_{xx}+I_{xy})(1-UI_0)} . \quad (13)$$

The integrals $I_\alpha(\alpha = x, xx, xy)$ are all related to the integral I_0, which diverges logarithmically for $|E| \le 8t$. From Eq. (12) for $\mathbf{Q}=\mathbf{0}$, one can easily show that

$$I_{xx} + I_{xy} = -\frac{E}{4t} I_x , \quad (14a)$$

$$I_x = \frac{1}{8t} - \frac{E}{8t} I_0 , \quad (14b)$$

$$I_0 = \frac{1}{E}\frac{2}{\pi} K\left[\frac{8t}{|E|}\right] , \quad (14c)$$

where $K(x)$ is the complete elliptic integral of the first kind. It is convenient to introduce quantities $S_\alpha = I_\alpha - I_0$, since the S_α are generally finite. After some manipulations we obtain

$$\frac{1}{2J} = \frac{4S_x}{1-1/UI_0} + \frac{2S_x^2}{I_0 - 1/U} - (B+2)S_x - BI_0 + \frac{2}{U-1/I_0} , \quad (15)$$

where $-4Bt = E + 8t$ is the binding energy. The critical value of J for forming a two-electron bound state may be found by setting the binding energy to zero, i.e., $B=0$; then $I_0 \to \infty$, $BI_0 \to 0$, and we get

$$\frac{J_{2c}}{t} = \frac{2}{1+8t/U} . \quad (16)$$

Therefore for the t-J model $(U\to\infty)$ we obtain $J_{2c} = 2t$. It is easy to show that this critical value J_{2c} is independent of the lattice size and dimensionality. Using Eqs. (13) and (14), the total energy E of the two-particle system, for the t-J model, can be obtained via equation

$$\frac{16t}{J} = \frac{\pi}{2}\frac{E/t}{K\left[\frac{8t}{|E|}\right]} - \frac{E}{t} . \quad (17)$$

Emery, Kivelson, and Lin,[3] have shown that the fully-phase-separated state is unstable to the transfer of single electron when $J \le 3.42t$. Since this value of J is greater than J_{2c}, we expected, as J is decreased, there would be an instability to form pairs before single particles. To investigate this problem we should compare the total energy, $E(J)$, of the two-particle system with $2E_1(J)$, where $E_1(J)$ is the total energy of single electron in the hole-rich phase. As shown in Ref. 3, $E_1(J) = -4t - 2BJ$, where $B = 0.584$. By solving Eq. (17) for $E(J)$, it can be shown that the instability to pairs occurs at $J \le 3.828t$. This raises the question whether the hole-rich phase may be regarded as a dilute gas of pairs of electrons when J is slightly less than $3.828t$ but above $J_{2c}(=2t)$, since a large cluster consisting of 3, 4, or more electrons may be formed. Indeed, for the t-J model, the interaction between electrons is attractive and it is well known[4] that systems with attractive interactions will collapse to arbitrarily high density when the dimension $d > 2$. In three dimensions, it is necessary to have some kind of short-range repulsion to stabilize the system. However, in two dimensions, an arbitrarily weak, purely attractive potential will bind a pair,[5] but the system may not collapse to higher density; i.e., a two-dimensional system may be able to form a low-density liquid of pairs. To investigate this possibility in the t-J model it is necessary to determine the critical values of J for the formation of three- or four-particle bound states and for condensation into a liquid. Since electrons attract each other only when they are on neighboring sites in the t-J model, for a square lattice it is easier to form a four-particle bound state than to form a three-particle state for purely geometrical reasons. The potential energy is $-J$ for 2 electrons bound together (1 bond) to form a dimer, $-\frac{3}{2}J$ for 3 electrons bound together (2 bonds), and $-3J$ for 4 electrons bound together (4 bonds) to form a square, respectively. Thus the average potential energy per electron is $-0.5J$ for two- and three-particle bound states, and $-0.75J$ for four-particle bound state. So it is easy to see that the instability to four-particle bound state occurs before that to three-particle bound state. We have studied the possibility of forming four-particle bound states by diagonalizing exactly the t-J model on various lattices up to 8×8 and then extrapolating to the infinite lattice. We determine the critical value of J_{4c} for a four-particle bound state by using the criterion that $E_4(N) = 2E_2(N)$, where $E_4(N)$ and $E_2(N)$ are the ground-state energies for four- and two-particle on a lattice of size N, respectively. In general, J_{4c} depends on the size of lattice. The following results were obtained: $J_{4c}(4\times 4) = (5.755\pm 0.005)t$, $J_{4c}(6\times 6) = (5.455\pm 0.005)t$, and $J_{4c}(8\times 8) = (5.30 \pm 0.05)t$. These values were plotted as functions of L^{-1}, where $N = L \times L$, in Fig. 1. The extrapolated value of J_{4c} for an infinite system is $(4.85 \pm 0.05)t$. Errors in the finite-lattice data arise from the fact that we do not have enough computer power to scan J in smaller steps ΔJ, especially for the 8×8 lattice. Our data fitted to $A + B/L$ extremely well, as can be seen from Fig. 1. We also tried to plot the data as functions of $1/N$ and they do not fit it well. The reason for the $1/L$ dependence is that while the potential energy does not depend on the size of lattice too much when the lattice is large enough such as 8×8, because of the short-range nature of interaction (nearest-neighbor attraction), the kinetic energy has $1/L$ dependence because of the cosine spectrum.

We may try to use perturbation theory to estimate the critical values of J_{2c} and J_{4c}. Starting with the two-electron system, we see that when $J \gg t$, two electrons will bind together to form a dimer with zeroth-order energy $-J$. By standard second-order-perturbation-theory arguments, we see that the leading kinetic energy contribution comes from the motion in which one of the electrons hops out of the dimer and later either this electron hops back or the other electron hops to join the first electron and then forms the dimer again. Higher-order terms can be obtained from Eq. (17), and we find that the total energy is

$$E_2 = -J - \frac{20t^2}{J} - \frac{48t^4}{J^3} - \cdots \quad (18)$$

For the four-electron system, in the limit $J \gg t$, the four electrons will bind together to form a square with potential energy $-3J$. To second order in t/J, there are only eight possible ways for one electron to hop out of the square and hop back. The energy difference is $3J/2$ so the total energy is, to second order in t/J,

$$E_4 = -3J - \frac{8t^2}{3J/2} = -3J - \frac{16t^2}{3J} \ . \quad (19)$$

Equating $E_4 = 2E_2$ we obtain $J_{4c} = \sqrt{104/3}t = 5.89t$, which is comparable to, but larger than, our numerical estimation of $J_{4c} = (4.85 \pm 0.05)t$, as expected.

In summary, our results indicate that there indeed exists a regime, $3.828 > J/t > 2$, in which the hole-rich phase contains a dilute gas of pairs of electrons. As J decreases from ∞, there is an instability to a four-particle bound state at $j/t = 4.85$. As J decreases further there is an instability to pairs at $J/t = 3.828$. Since the pairs are bosons, they probably form a superfluid at low temperatures. As J/t is decreased further from 3.828, the density of pairs may build up sufficiently for the system to become a BCS superconductor, but there must be a crossover to a different state at least by $J = 2t$ (where the pairs unbind) since a necessary and sufficient condition for BCS pairing in a dilute gas is that there is a two-body bound state.[5]

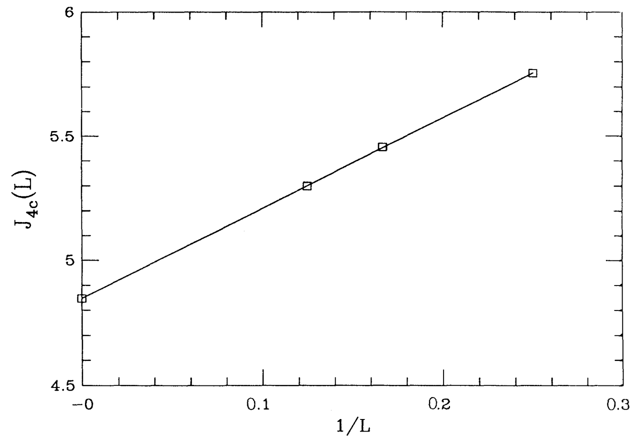

FIG. 1. Critical value J_{4c} (see the text for definition) as function of L, where $N = L \times L$ is the size of square lattice. Estimation errors are smaller than symbols presented.

I am very grateful to V. Emery and S. Kivelson for suggesting this problem to me and for useful contributions. I thank D. Campbell for constantly supporting my research at CNLS. This work is supported by Los Alamos National Laboratory and the U.S. DOE Office of Energy Research.

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