Bound states of electrons (holes) on a square lattice and their superfluidity

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An elementary model of the Hubbard type is proposed and used to study the spectrum of two-particle electron states. Conditions under which bound states coexist with unbound states are found. Superfluidity criteria are discussed.

Experiments[1] show that the basic properties of the high-temperature superconductors are determined by the electrons of copper-oxygen (CuO_2) layers. The holes which arise as a result of doping belong to an oxygen band. This circumstance is taken into account systematically in a generalized Hubbard model[2,3] which we have used previously[4] to study the spectrum of hole excitations. In the case of a pronounced hybridization of p and d states, the generalized Hubbard model reduces to the ordinary model with renormalized values of the Coulomb energy U and the hopping energy t, as was pointed out in Ref. 3. The unit cell $\mathbf{r}$ consists in this case of one copper ion and its oxygen surroundings. A hole localized at a copper ion forms a nearly singlet state with a free hole, which is smeared over the oxygen surroundings of the given ion. The "hops" of this complex form a hole band.[4] This version can be described approximately by the Hamiltonian

$$\mathcal{H} = -\sum_{\langle \mathbf{r},\mathbf{r}'\rangle,\sigma} a^{+}_{\mathbf{r}\sigma} a_{\mathbf{r}'\sigma} \left(t + \tau\left(n_{\mathbf{r}-\sigma} + n_{\mathbf{r}'-\sigma}\right)\right) + \sum_{\mathbf{r}} U n^{\uparrow}_{\mathbf{r}} n^{\downarrow}_{\mathbf{r}}. \qquad (1)$$

Here the Fermi operators $a_{\mathbf{r}\sigma}$ ($a^{+}_{\mathbf{r}\sigma}$) annihilate (create) a hole in cell $\mathbf{r}$. The notation $\langle \mathbf{r},\mathbf{r}\rangle$ is adopted for nearest cells. The quantity τ describes the change in the hopping amplitude t which stems from the formation or decay of a two-particle state, characterized by an energy U, in one cell. In our approach, the "Hubbard" energy U is of course on the order of t, as τ is. We will be discussing the case of a slightly filled band

$(nU \ll t)$, in which we can avoid the Hubbard-gap problem. The one-particle states of Hamiltonian (1) have the spectrum

$$\epsilon(R) = -2t(\cos(K_x) + \cos(K_y)) \tag{2}$$

(we are assuming a unit lattice constant). The spectrum of singlet two-particle states $E(\mathbf{Q})$ with a resultant wave vector $\mathbf{Q}$ is found from the equation

$$\theta U + (1-\theta)E = W^{-1}(E; \mathbf{Q}), \tag{3}$$

where $\theta = (1 + \tau/t)^{-2}$, and

$$W(E; \mathbf{Q}) = \int d^2K (E - \epsilon(K) - \epsilon(K - \mathbf{Q}))^{-1} / (2\pi)^2, \tag{4}$$

Equation (3) can be derived by solving the two-particle Schrödinger equation or by determining the poles of the two-particle Green's function. It is easy to see that Eq. (3) is symmetric with respect to the simultaneous substitutions $U \to -U$ and $E \to -E$ and that the spectrum $E(\mathbf{Q})$ is specified completely by its values in the region $\pi \geqslant Q_y \geqslant Q_x \geqslant 0$. Equation (3) contains a continuous spectrum of solutions, which corresponds to two-particle unbound states with a momentum $\mathbf{Q} = \mathbf{k}_1 + \mathbf{k}_2$ and energies $E = \epsilon(\mathbf{k}_1) + \epsilon(\mathbf{k}_2)$. These solutions are bounded by the surfaces

$$E = \pm A(\mathbf{Q}),\ A(\mathbf{Q}) = 4t(|\cos(Q_x/2)| + |\cos(Q_y/2)|). \tag{5}$$

Figure 1 shows the cross section $Q_x = Q_y$. The hatching shows the region of unbound states. In addition to a continuum, Eq. (3) can have discrete solutions $E(\mathbf{Q})$ at a fixed $\mathbf{Q}$. Corresponding to these states are wave functions which decay exponentially with increasing distance between particles. If $E(\mathbf{Q}) < -8t$, this is a stable two-particle state. If $E(\mathbf{Q}) > -8t$, the bound state is metastable and may decay into unbound states of the continuum in a process in which momentum (energy) is transferred to a third particle or to a phonon (an analog of an exciton in a semiconductor).

In the region in which bound states exist, $|E| > A(\mathbf{Q})$, the quantity W^{-1} is nonzero and is given by

$$W^{-1}(E; \mathbf{Q}) = 0.5\pi\, \mathrm{sign}(E)(E^2 - B^2)^{1/2}\, \mathbf{K}^{-1}(R), \tag{6}$$

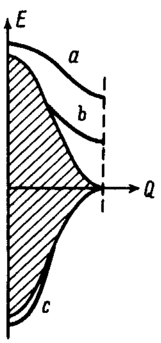

FIG. 1.

where $B = 4t(|\cos(Q_x/2)| - |\cos(Q_y/2)|)$, $R^2 = (A^2 - B^2)/(E^2 - B^2)$, and $\mathbf{K}(R)$ is the complete elliptic integral. It is easy to see that there always exists a discrete solution of Eq. (3) at the point $\mathbf{Q} = (\pi,\pi)$:

$$E(\pi,\pi) = U.$$

For definiteness we assume $U > 0$ and $\theta > 1$. The latter assumption means that the amplitude $(t + \tau)$ for the coalescence of two particles into a single cell is smaller than the hopping amplitude t. Under the inequality

$$U > U_0 = 8t\ (1 - \theta^{-1}) \tag{7}$$

there will then be a mode α of discrete states which is above the continuum for all $\mathbf{Q}$ (line a in Fig. 1). The spectrum of two-particle excitations at $U > 8t$ is a two-band spectrum, while the spectrum of one-particle excitations, (2), remains a single-band spectrum even in the limit $U \gg t$ (but in $U < t$).

If condition (7) does not hold, discrete mode b (line b in Fig. 1) will merge with the continuum along the contour line

$$E_c\ (\mathrm{Q}) = A_c\ (\mathrm{Q}) = U\,(1 - \theta^{-1}). \tag{8}$$

Under the condition $\theta < 1$, Eq. (3) has an isolated mode of type a; in addition, at $0 < U < |U_0|$ it has yet another discrete mode, c (line c in Fig. 1), which merges with the continuum along line (8), but in this case the condition $E_c < 0$ holds! This mode has a minimum at the point (0,0):

$$E\,(0,\ 0) = -8t - \Delta,\ \Delta = 64t\,\exp\,(-1/\lambda). \tag{9}$$

If U is close to $|U_0|$, we have $\lambda = \pi^{-1}(1 - \theta)(1 - \mathrm{U}/|\mathrm{U}_0|)$, and the effective mass of the bound excitation is $m \simeq t^{-1}$.

Stable bound states also exist for a local single-cell attraction if $\theta < 1$ for all $U < 0$ and if $\theta > 1$ for $U < -|U_0|$. The picture shown in Fig. 1 for this case should be reflected in the (Q_x, Q_y) plane for this case.

All of the bound two-particle states which we have mentioned here correspond to Bose statistics, and at low temperatures $T < T_c \approx nT$ they may form a superfluid gas. The analysis above is valid as long as the characteristic kinetic energy ($\propto nT$) is small in comparison with the binding energy Δ or, equivalently, as long as the size of the composite Bose particles is much smaller than the distance between these particles. In the opposite case, we would need to consider the deformation of the bound state caused by the Fermi filing of one-particle states. Equations (3) and (4) change in this case:

$$\theta U + (1 - \theta)E + 4\tau^2 t^{-1} I_1 \theta = W^{-1}\ , \tag{3'}$$

where $\theta = (1 + \tau t^{-1} I_0)^{-2}$, $W = (2\pi)^{-2} \int d^2R(E - \epsilon(\mathbf{k}) - \epsilon(\mathbf{k} - \mathbf{Q}))^{-1}$,

$$I_0 = (2\pi)^{-2} \int\ d^2K,\ I_1 = (2\pi)^{-2} \int\ d^2K(\cos(K_x) + \cos(K_y)). \tag{4'}$$

The integration in (4') is over the region $\epsilon(\mathbf{k}) > \epsilon_F$ and $\epsilon(\mathbf{k} - \mathbf{Q}) > \epsilon_F$. A detailed

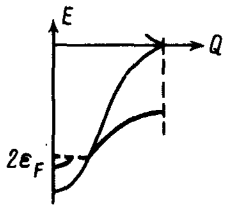

FIG. 2. One type of deformation of mode b in the case $U<0$.

analysis of a Cooper problem of this type will be published separately (see also Fig. 2). It follows from this analysis that, in particular, the binding energy of a Cooper pair decreases for mode c and increases for mode b (if $U<0$) with increasing density n.

Finally, we use the BCS theory to analyze the problem. In the momentum representation, Hamiltonian (1) is written

$$\mathcal{H}=\sum_{\mathbf{k}} \xi(\mathbf{k})\, a^{+}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + (2N)^{-1} \sum_{\{\mathbf{k}\}} \lambda(\{\mathbf{k}\}) a^{+}_{\mathbf{k}_1\sigma} a^{+}_{\mathbf{k}_2-\sigma} a_{\mathbf{k}_3-\sigma} a_{\mathbf{k}_4\sigma}, \tag{10}$$

where $\xi(\mathbf{k})=\epsilon(\mathbf{k})-\mu$, $\lambda(\{\mathbf{k}\})=U+\Sigma_i \tau_{\mathbf{k}_i}$, and $\tau_{\mathbf{k}}=-2\tau(\cos(K_x)+\cos(K_y))$. The equation for the gap is well known:

$$\Delta_{\mathbf{k}}=-(2N)^{-1}\sum_{\mathbf{k}_1} \Delta_{\mathbf{k}_1} \lambda(\mathbf{k},\mathbf{k},\mathbf{k}_1,\mathbf{k}_1) E^{-1}(\mathbf{k}_1)\tanh(E(\mathbf{k}_1)/(2T)), \tag{11}$$

where $E(\mathbf{k})=(\xi^2(\mathbf{k})+\Delta^2(\mathbf{k}))^{1/2}$ is the spectrum of elementary excitations. From Eq. (11) we find $\Delta_{\mathbf{k}}=D_0+D_1\tau_{\mathbf{k}}$.

Since the parameters (U,t,τ) may be of the same order of magnitude in our model, at $T=0$ we cannot restrict the solution of Eq. (11) to the customary logarithmic approximation. In the limit $T\to T_c$, however, the gap vanishes, and the customary logarithmic approximation becomes legitimate. In this case we have $D_0=D_1(U+2\tau_F)/2, \tau_F=\mu\tau/t$, and

$$1=-(2N)^{-1}(U+4\tau_F)\,\Sigma_{\mathbf{k}} E^{-1}(\mathbf{k})\tanh(E(\mathbf{k})/(2T)). \tag{12}$$

We see that the equation for the gap has its standard form; the role of an effective interaction constant is played by the value of λ at the Fermi surface:

$$\lambda_{\text{eff}}=U+4\mu\tau/t. \tag{13}$$

A solution of Eq. (13) exists if $\lambda_{\text{eff}}<0$. If $U<0$, we would need $\mu<|U|t/(4\tau)$. In other words, the $\epsilon(\mathbf{k})$ band can in principle be more than half-filled. If, on the other hand, $U>0$, the Fermi energy should be negative, and the relation $|\mu|>U\,t/(4\tau)$ should hold. Since $|\mu|$ cannot be greater than $4t$ in this model, a superfluid state exists in the case $U>0$ only if

$$U<16\tau. \tag{14}$$

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