Journal of Theoretical Physics

Founded and Edited by M. Apostol **22** (1997)

ISSN 1453-4428

η-superconductivity is an unstable π-superconductivity

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Abstract

The energy spectrum of the one-pair states of electrons with opposite spins is computed for the Hubbard model in a cubic lattice. It is shown that the one-pair energy spectrum of the Hubbard hamiltonian consists of the free-electron band and a band of collective modes. The eigenstate introduced by Yang (C. N. Yang, Phys. Rev. Lett. **63** 2144 (1989)) in connection with the so-called η-pairing is such a collective mode; this mode is unstable, in the sense that it may decay on one-pair states of lower energy.

In a recent publication, Yang[1] introduced the notion of η-pairing in connection with a certain eigenstate of a typical Hubbard model.The model is described by the hamiltonian

$$H = \sum_k \varepsilon_k \left(a_k^+ a_k + b_k^+ b_k \right) + U \sum_r a_r^+ a_r b_r^+ b_r \quad , \tag{1}$$

where $a_k(b_k)$ are the fermion operators for the electron states of wavevectors k and spin up (down), r denotes the lattice sites, U is the interaction strength, and

$$\varepsilon_k = \varepsilon \left(6 - 2\cos k_x - 2\cos k_y - 2\cos k_z \right) \quad , \quad \varepsilon > 0 \quad , \tag{2}$$

are the free energy levels of the one-electron states, corresponding, for convenience, to a cubic lattice. Yang′s eigenstate

$$\mid \psi_0(\pi)\rangle = \frac{1}{\sqrt{N}} \sum_r e^{i\pi r} a_r^+ b_r^+ \mid 0\rangle \quad , \tag{3}$$

where N is the total number of lattice sites, consists of a superposition of electron pairs with opposite spins, has the energy $12\varepsilon + U$ and momentum π, and exhibits off-diagonal long-range order. The operator acting in (3) upon the vacuum $\mid 0\rangle$ is denoted by η^+, and, by applying it repeatedly, one can construct a macroscopic eigenstate of both the energy and the momentum; in addition, for a large enough negative U this eigenstate is sufficiently low in energy, so that it may be tempting to associate it with a true superconducting state. However, as Yang points out, there exist mixing states, as, for instance, those constructed from Cooper′s state

$$\mid \Phi_0\rangle = \frac{1}{\sqrt{N}} \sum_r a_r^+ b_r^+ \mid 0\rangle \quad , \tag{4}$$

whose average energy is equal with Yang′s eigenenergy, whence it follows that Yang′s eigenstate is not the ground-state. Yang suggested that this eigenstate would be metastable, by decaying on two-electron states lower in energy via a precursor tunneling through two excited one-pair states.

We compute in this paper the energy spectrum of the one-pair states of electrons with opposite spins, and show that Yang′s eigenstate is unstable with respect to one-pair states. In addition, we suggest that η-superconductivity would be more properly referred to as a π-superconductivity. We show also that the one-pair energy spectrum of the Hubbard hamiltonian consists of the free-electron band and a band of collective modes.

Without any loss of generality we may take

$$\mid \varphi_k(q)\rangle = \frac{1}{\sqrt{2}}\left(a_k^+ b_{q-k}^+ \pm b_k^+ a_{q-k}^+\right) \mid 0\rangle \tag{5}$$

as the basic set of one-pair states of electrons with opposite spins; both k and q in (5) run over the entire Brillouin zone, and $q-k$ is also reduced, whenever necessary, to the Brillouin zone. These states are orthogonal to each other and have a well-defined momentum q. They correspond to a singlet or triplet pair of electrons, and we can use them as the basic set for the Hubbard hamiltonain since this hamiltonian preserves the spin. These basic states have a twofold spin degeneracy, and we shall keep it in mind, without, however, write it explicitly. Applying the hamiltonian (1) on these states we obtain

$$H \mid \varphi_k(q)\rangle = (\varepsilon_k + \varepsilon_{q-k}) \mid \varphi_k(q)\rangle + \frac{U}{N}\sum_{k'} \mid \varphi_{k+k'}(q)\rangle \quad , \tag{6}$$

where one can see that the hamiltonian does not change the momentum q. Consequently we can look for the eigenstates of the form

$$\mid \psi_k(q)\rangle = \sum_k c_k \mid \varphi_k(q)\rangle \quad , \tag{7}$$

in each q-sector, where the coefficients c_k are solutions of the system of equations

$$(\varepsilon_k + \varepsilon_{q-k} - \lambda)\, c_k + \frac{U}{N}\sum_k c_k = 0 \quad , \tag{8}$$

λ being the eigenvalues.

For $q=\pi$ one may check easily that $c_k^r = \exp(ikr)/\sqrt{N}$, the eigenstates are

$$\mid \psi_r(\pi)\rangle = \frac{1}{\sqrt{N}}\sum_k e^{ikr} \mid \varphi_k(\pi)\rangle \quad , \tag{9}$$

and the eigenvalues are given by $\lambda_0(\pi) = 12\varepsilon + U$, and a degenerate band $\lambda_r = 12\varepsilon$ for $r \neq 0$. In addition, we see easily that $\mid \psi_0(\pi)\rangle$ given by (9) for the singlet case is Yang′s eigenstate (3). We note also that the degenerate band $\lambda_r = 12\varepsilon$ for $r \neq 0$ is actually the two-electron band corresponding to the free electron states with opposite spins.[2]

For $q \neq \pi$ we obtain from (8)

$$f(\lambda) = -\frac{U}{N}\sum_k \frac{1}{\varepsilon_k + \varepsilon_{q-k} - \lambda} = 1 \quad . \tag{10}$$

The analysis of this equation for λ is classical. In the limit of large N it has a band of solutions in the pair continuum, which extends from $\varepsilon_m(q) = \min_k(\varepsilon_k + \varepsilon_{q-k})$ to $\varepsilon_M(q) = \max_k(\varepsilon_k + \varepsilon_{q-k})$, and a collective mode. The eigenvalues in the pair-continuum band are twofold degenerate. We describe these solutions below. Beforehand, we note, however, that

$$\begin{aligned} \varepsilon_m(q) &= 12\varepsilon\left[1 - \tfrac{1}{3}\left(\cos q_x/2 + \cos q_y/2 + \cos q_z/2\right)\right] \quad , \\ \varepsilon_M(q) &= 12\varepsilon\left[1 + \tfrac{1}{3}\left(\cos q_x/2 + \cos q_y/2 + \cos q_z/2\right)\right] \quad , \end{aligned} \tag{11}$$

as follows from a straightforward analysis of the function $\varepsilon_k + \varepsilon_{q-k}$ with ε_k given by (2).

The pair-continuum band given by equation (10) has the eigenstates

$$\mid \psi_k(q)\rangle = \mid \varphi_k(q)\rangle \tag{12}$$

in the limit of large N,[3] corresponding to the eigenvalues $\lambda_k(q) = \varepsilon_k + \varepsilon_{q-k}$. We note that this pair-continuum band is actually the two-electron band of free electron states with opposite spins. We note also that there exists a mixing singlet state

$$\mid \Phi_q\rangle = \frac{1}{\sqrt{N}}\sum_k \mid \varphi_k(q)\rangle \tag{13}$$

whose average energy is $12\varepsilon + U$, *i.e.* it is equal with the energy of Yang's eigenstate $\mid \psi_0(\pi)\rangle$ and Cooper's state $\mid \Phi_0\rangle$. For $U > 0$ Yang's eigenvalue $12\varepsilon + U$ is higher than the upper limit 12ε of the free electron band, so that Yang's eigenstate is unstable in this case with respect to the decay on the one-electron continuum.

The collective mode can be computed easily for $|U| \gg 12\varepsilon$ by expanding $f(\lambda)$ in (10) in powers of $(\varepsilon_k + \varepsilon_{q-k})/\lambda$. The calculations are straightforward and one obtains

$$\lambda_0(q) = 12\varepsilon + U + 8\left(\cos^2 q_x/2 + \cos^2 q_y/2 + \cos^2 q_z/2\right)\cdot\frac{\varepsilon^2}{U} + ..., \tag{14}$$

corresponding to the singlet eigenstate

$$\mid \psi_0(q)\rangle = \frac{1}{\sqrt{N}}\sum_k\left(1 + \frac{\varepsilon_k + \varepsilon_{q-k} - 12\varepsilon}{U} + ...\right)\mid \varphi_k(q)\rangle \quad . \tag{15}$$

The picture of the eigenvalues given by (10) for $U < -12\varepsilon$ is shown in Fig.1 for $q \neq \pi$. We note that Yang's eigenenergy $12\varepsilon + U$ (and the average energy of the mixing state given by (13)) is always lower or higher than $\lambda_0(q)$ for $U > 0$ or, respectively, $U < 0$, for any $q \neq \pi$. The ground-state is $\mid \psi_0(0)\rangle$, for $U < 0$, and one can see that it is made of a superposition of Cooper's pairs. In the case of large, negative U we see that the ground-state energy is $\lambda_0(0) = 12\varepsilon + U + 8\varepsilon^2/U + ...$, corresponding to $\mid \psi_0(0)\rangle$ given by (15). The energy spectrum is shown schematically in Fig.2 for $U < -12\varepsilon$.

The collective modes $\mid \psi_0(q)\rangle$ are made of superpositions of singlet electron pairs and possess off-diagonal long-range order. They admit, in principle, a macroscopic occupancy. In addition,

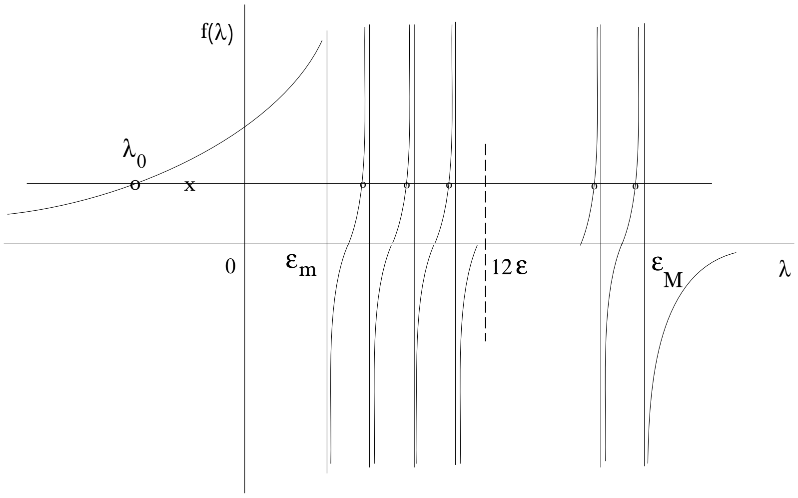

Figure 1: Graphical representation of equation $f(\lambda) = 1$ for $U < -12\varepsilon$, with $f(\lambda)$ given by (10). The eigenvalues in the pair continuum are indicated by small, open circles; the cross represents the average energy of the mixing state $\mid \Phi_q\rangle$.

for $U < 0$ they are the "ground-states" of their own q-sectors, so that they may be called "superconducting" states. Yang′s eigenstate is a member of this group of states, corresponding to $q = \pi$, so that η-superconductivity would be better referred to as a π-"superconductivity". However, for $U < 0$ these states are unstable with respect to the true ground-state $\mid \psi_0(0)\rangle$, which is made of a superposition of Cooper′s pairs. The macroscopic occupancy of this ground-state differs from the BCS superconducting state in that it corresponds to a well-defined number of electrons, while, on the contrary, in the latter.the number of electrons is not fixed; as it is well known, the BCS state has a phase coherence and a true symmetry breaking. The superconducting transition to $\mid \psi_0(0)\rangle$ for $U < 0$ proceeds by a Bose-Einstein condesation.

Finally, we note that the hamiltonian given by (1) has also one-electron eigenstates of energy ε_k, corresponding to the free electron states with parallel spins. As we remarked, the pair-continuum bands found above correspond in fact to the two-electron bands of free electron states with opposite spins. Therefore, one may conclude that the one-pair energy spectrum of the Hubbard hamiltonian consists of the free one-electron states ε_k (which extend from 0 to 12ε) and a band of collective modes $\lambda_0(q)$. The latter is always above $\varepsilon_M(q)$ (and 12ε) for $U > 0$, and below $\varepsilon_m(q)$ (and ε_q) for $U < 0$. In the first case it is unstable with respect to the one-electron continuum, while in the second case it is unstable with respect to the ground-state $\mid \psi_0(0)\rangle$. The physical picture is that electrons have enough room to avoid each other for $U > 0$, thus behaving practically as free electrons, while they pair themselves in spin singlets with opposite momenta (Cooper′s pairing) for $U < 0$, in order to take advantage of the attraction.

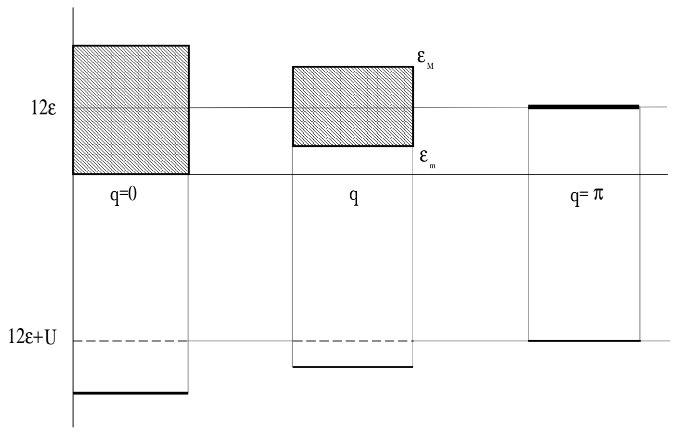

Figure 2: A schematic representation of the energy spectrum of the one-pair states of electrons with opposite spins in various q-sectors for $U < -12\varepsilon$. The shaded areas correspond to the pair continuum, the solid lines at the bottom of each sector represent the collective modes, and the dashed lines above the collective modes represent the mixing states $\mid \Phi_q\rangle$. The collective mode in the π-sector is Yang$'$s eigenstate, and the one in the sector $q = 0$ is the ground state.

References

[1] C. N. Yang, Phys. Rev. Lett. **63** 2144 (1989).

[2] This degenerate band consists of Yang$'$s excited one-pair states, see Ref.1.

[3] The $1/N$-corrections to these eigenstates and eigenvalues are given by

$$\mid \psi_k(q)\rangle = \mid \varphi_k(q)\rangle + \frac{U}{N}\sum_{k'\neq k}\left(\varepsilon_k + \varepsilon_{q-k} - \varepsilon_{k'} - \varepsilon_{q-k'}\right)^{-1} \mid \varphi_{k'}(q)\rangle \quad ,$$

and

$$\lambda_k(q) = \varepsilon_k + \varepsilon_{q-k} + U/N \quad .$$