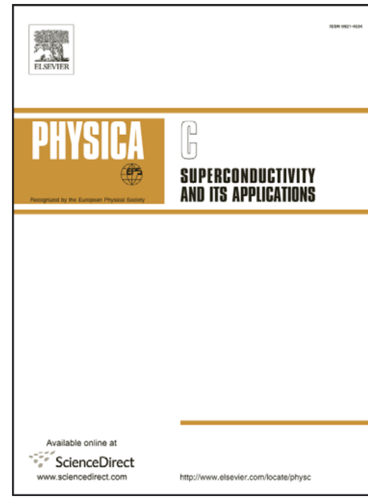

On Electron Pairing In a Periodic Potential

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On Electron Pairing In a Periodic Potential

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A model Hamiltonian is proposed, based on the assumption that two electrons with the same group velocity effectively attract each other, to examine the existence of unconventional electron pairs formed by electrons in a strong periodic potential.

Despite intensive experimental and theoretical research the mechanism responsible for high temperature superconductivity[1] is yet not clear. Among different theoretical approaches there is a view that formation of electron pairs is a natural property of interacting electrons immersed in a strong periodic potential[2,3]. In particular, as one of the possibilities a hole-electron paring mechanism[4] is suggested, where an electron is paired with a hole traveling in space in opposite direction. As a possible extension of the hole-electron paring we can assume that electron pairs are formed by electrons traveling *with the same group velocity*.

Based on the assumptions above, we write a model Hamiltonian in the following form:

$$H = \sum_{p\sigma} (\varepsilon_p - \mu) a^+_{p\sigma} a_{p\sigma} + U , \qquad \varepsilon_p = -t(\cos p_x + \cos p_y) . \tag{1}$$

In Eq. (1) the first term represents the kinetic energy of electrons in a 2D square lattice written in the tight-binding approximation; $t > 0$ is hopping integral. Here and throughout the letter we assume the lattice constant, the Plank's constant, and the Boltzmann's constant are equal to unity. For all electrons momenta lie in the first Brillouin zone $-\pi < p_{x,y} < \pi$; μ is a chemical potential introduced in the Hamiltonian as a Lagrange multiplier; $a^+_{p\sigma}$ and $a_{p\sigma}$ are creation and annihilation operators for an electron with momentum $\boldsymbol{p} = (p_x, p_y)$ and spin component σ ($\sigma = +, -$). The second term U in Eq. (1) describes an effective attraction between electrons with the same group velocity.

For an electron with momentum $\boldsymbol{p} = (p_x, p_y)$ and kinetic energy $\varepsilon_{\boldsymbol{p}} = -t(\cos p_x + \cos p_y)$ there might exists three more electrons with the same group velocity $v_{\boldsymbol{p}} = \nabla \varepsilon_{\boldsymbol{p}}$, namely, $\boldsymbol{p}^* = (\pi \cdot sgn(p_x) - p_x, \pi \cdot sgn(p_y) - p_y)$, $\boldsymbol{p}^{/} = (p_x, \pi \cdot sgn(p_y) - p_y)$, $\boldsymbol{p}^{//} = (\pi \cdot sgn(p_x) - p_x, p_y)$ ($sgn(p_{x,y})$ is the signum function).

Thus, in general, there might be formed a cluster of four electrons with the same group velocity.

In this letter we limit ourselves to the simplest interaction term

$$U = -\frac{W}{N} V^+ V, \qquad V^+ = \sum_{\boldsymbol{p}} a^+_{\boldsymbol{p}\uparrow} a^+_{\boldsymbol{p}*\downarrow}. \tag{2}$$

In Eq. (2) N is the number of sites, $W > 0$ is a coupling constant for paired electrons, and the summation runs over the first Brillouin zone.

Let us introduce a Bogolyubov-like canonical transformation

$$a_{\boldsymbol{p}\uparrow} = u_{\boldsymbol{p}} b_{\boldsymbol{p}\uparrow} - v_{\boldsymbol{p}} b^+_{\boldsymbol{p}*\downarrow}, \quad a_{\boldsymbol{p}\downarrow} = u_{\boldsymbol{p}} b_{\boldsymbol{p}\downarrow} + v_{\boldsymbol{p}} b^+_{\boldsymbol{p}*\uparrow}, \quad u_{\boldsymbol{p}} = u_{\boldsymbol{p}*} > 0, \quad v_{\boldsymbol{p}} = v_{\boldsymbol{p}*} > 0, \quad u^2_{\boldsymbol{p}} + v^2_{\boldsymbol{p}} = 1. \tag{3}$$

With the means of transformation (3), using essentially a mean-field approximation regular for such a procedure[5], after diagonalization of Hamiltonian (1)-(2), we obtain energy levels ($n_{p\sigma} = 0, 1$)

$$E = -2\mu\sum_{p} v_p^2 + \sum_{p,\ \sigma}(\varepsilon_p - \mu(u_p^2 - v_p^2))n_{p\sigma} - \frac{W}{N}\left[\sum_{p} u_p v_p (1 - n_{p+} - n_{p-})\right]^2. \quad (4)$$

Equation (4) is a direct equivalent of Eq. 39.10 in the well know textbook by L.P. Pitaevskii and E.M. Lifshitz[6].

Equation (5)

$$-2\mu u_p v_p = (u_p^2 - v_p^2)\frac{W}{N}\sum_{p} u_p v_p (1 - n_{p+} - n_{p-}) \quad (5)$$

insures the elimination of non-diagonal terms in Hamiltonian (4), and also minimizes the free energy of the system. This equation defines parameters u_p and v_p of canonical transformation (3).

For the number of electrons $N_e = -\frac{\partial E}{\partial \mu}$ we find

$$N_e = 2\sum_{p} v_p^2 + \sum_{p}(u_p^2 - v_p^2)(n_{p+} + n_{p-}). \quad (6)$$

After elementary transformations we obtain

$$u = \frac{1}{\sqrt{2}}\sqrt{1 - \frac{2\mu}{\Delta}}, \qquad v = \frac{1}{\sqrt{2}}\sqrt{1 + \frac{2\mu}{\Delta}}, \qquad \Delta = \frac{W}{N}\sum_{p}(1 - n_{p+} - n_{p-}). \quad (7)$$

Solution (7) exist only when $\frac{2|\mu|}{|\Delta|} < 1$.

Combining Eq. (6) and (7) we find

$$\mu = \frac{N_e - N}{N} * \frac{W}{2}. \quad (8)$$

For elementary excitations with distribution $n_p = [1 + \exp(\frac{\omega_p}{T})]^{-1}$ we obtain the spectrum

$$\omega_p = \varepsilon_p - \mu(u^2 - v^2) + 2\frac{W}{N}u^2v^2\sum_p(1 - n_{p+} - n_{p-}) = \varepsilon_p + \frac{\Delta}{2}. \tag{8}$$

When $\frac{W}{4t} > 1$ ($\varepsilon_p + \frac{W}{2} > 0$) there are no excitations in the ground state, and expression (8) shows the existence of gap $W/2$ in the excitation spectrum. The pairing function $< a^+_{p+} a^+_{p^*+} >= -uv \neq 0$ shows the existence of electron pairs. However, those pairs cannot be responsible for superconductivity; for example, they exist even at the half filling ($u = v = 1/\sqrt{2}$ when $N_e = N$). This leads us to conclude that model Hamiltonian (1)-(2) does not describe properties of HTSC. The further analysis should show if an inclusion of four-electron clusters and a more realistic interaction term would support the notion of a hole-electron paring[4] in high temperature super conductors.

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