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Abstract

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ON ONE MODEL OF A SUPERCONDUCTOR WITH PAIRS IN A p-STATE

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In a recent preprint, Balian and Werthamer ([1]) proposed a model of a superconductor in which the condensate pairs are in states with orbital angular momentum $l = 1$. The model is described by a Hamiltonian of the form

$$H = \sum_k \xi_k \left(a_k^+ a_k + b_k^+ b_k\right) -$$

$$-\frac{1}{2V} \sum_{k,k'} J(k,k') \left(a_k^+ a_{-k}^+ a_{-k'} a_{k'} + 2a_k^+ b_{-k}^+ b_{-k'} a_{k'} + b_k^+ b_{-k}^+ b_{-k'} b_{k'}\right). \qquad (1)$$

Here ξ_k is the particle energy measured from the Fermi sphere; a_k^+, a_k, b_k^+, b_k are the creation and annihilation operators of Fermi particles with spin $1/2$ and $-1/2$, respectively; $J(k,k')$ is the "potential" of the direct interaction; V is the volume of the system. It is assumed that $J(k,k')$ differs from zero only in a layer near the Fermi sphere of thickness 2Λ, and within this layer is a function of the angle between the vectors k and k', having the form

$$J(k,k') = \frac{4\pi}{3}\, g \sum_{m=-1}^{1} Y_{1,m}(\hat{k}) Y_{1,m}^*(\hat{k}'), \qquad (2)$$

where $\hat{k} = k/|k|$.

This model, as is clear from (1), describes pair correlations between particles with opposite momenta and with total spin projection on the z-axis equal to $1, 0$, and -1. An interesting feature of this model is that it has a solution with an isotropic gap, corresponding to the minimum of the free energy. Another important feature of the model is its exact solvability for an infinite volume of the system. The latter can be proved analogously to how this is done for the usual BCS model ([2,3]), and is connected with the fact that the interaction Hamiltonian contains one fewer summation than the unreduced one.

In ([1]) the theory was constructed on the basis of a variational principle. An interesting result of the authors is a simple explanation, within the framework of this model, of the Knight shift. However, the mathematical treatment was carried out in an unjustifiably complicated way, and, most importantly, too broad a set of solutions was obtained, of which only a certain class has physical meaning. In the present note we formulate the necessary and sufficient condition that singles out the "physical" solutions, and prove that they are asymptotically exact as $V \to \infty$.

We shall use the technique of two-time Green' s functions (for the definition and basic notation, see the review ([4])). Averaging will be performed over the ground state, and the averages will be understood in the sense of the quasiaverages of N. N. Bogolyubov ([5]), i.e., we must assume that sources of pairs are included in the Hamiltonian (also violating the spin conservation law), and that after carrying out the limiting transition $V \to \infty$ the sources are made to tend to zero. Thus, the following Green' s functions are introduced:

$$\begin{aligned} G_{k\uparrow}(t-t') &= \langle\langle a_k(t); a_k^+(t')\rangle\rangle, \quad F_{k\uparrow}(t-t') = \langle\langle a_{-k}^+(t); a_k^+(t')\rangle\rangle, \\ G_{k\downarrow}(t-t') &= \langle\langle b_k(t); a_k^+(t')\rangle\rangle, \quad F_{k\downarrow}(t-t') = \langle\langle b_{-k}^+(t); a_k^+(t')\rangle\rangle. \end{aligned} \tag{3}$$

Along with these functions one must introduce the functions obtained from those written above by the replacement $a^+(t') \to b^+(t')$, but there is no need to consider them explicitly.

The equations of motion can be written in compact form if we introduce the notation:

$$c_k^{(1)} = -\frac{1}{V}\sum_{k'} J(\mathbf{k},\mathbf{k}')\, b_{-\mathbf{k}'} a_{k'},$$

$$c_k^{(2)} = \frac{1}{V}\sum_{k'} J(\mathbf{k},\mathbf{k}')\, a_{-\mathbf{k}'} a_{k'}, \qquad c_k^{(3)} = -\frac{1}{V}\sum_{k'} J(\mathbf{k},\mathbf{k}')\, b_{-\mathbf{k}'} b_{k'}. \tag{4}$$

It is easy to verify that these operators, and the conjugate operators to them, commute with one another and with the particle operators as $V \to \infty$. On this basis we may regard them, up to terms vanishing in the limiting transition, as c-numbers equal to the limits of their averages over the ground state. Denoting these averages respectively by $\Delta_{k\downarrow\uparrow}$, $\Delta_{k\uparrow\uparrow}$, and $\Delta_{k\downarrow\downarrow}$, and also introducing the matrix notation

$$\hat{G}_k = \begin{pmatrix} G_{k\uparrow} \\ G_{k\downarrow} \end{pmatrix}, \qquad \hat{F}_k = \begin{pmatrix} F_{k\uparrow} \\ F_{k\downarrow} \end{pmatrix}, \qquad \hat{\Delta}_k = \begin{pmatrix} \Delta_{k\uparrow\uparrow} & \Delta_{k\downarrow\uparrow} \\ \Delta_{k\uparrow\downarrow} & \Delta_{k\downarrow\downarrow} \end{pmatrix}, \qquad \hat{I} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{5}$$

we obtain, for the Fourier transforms of the Green functions, the system of equations

$$\begin{aligned} (\omega - \xi_k)\hat{G}_k(\omega) - \hat{\Delta}_k \hat{F}_k(\omega) &= \frac{1}{2\pi}\hat{I}, \\ -\hat{\Delta}_k^* \hat{G}_k(\omega) + (\omega + \xi_k)\hat{F}(\omega) &= 0. \end{aligned} \tag{6}$$

The solution of the dispersion equation leads to two branches in the spectrum of one-particle excitations

$$\omega_k^2 = \xi_k^2 + \frac{1}{2}\left\{\mathrm{Sp}\,\hat{\Delta}_k\hat{\Delta}_k^* \pm \sqrt{\left(\mathrm{Sp}\,\hat{\Delta}_k\hat{\Delta}_k^*\right)^2 - 4\det\hat{\Delta}_k\hat{\Delta}_k^*}\right\}. \tag{7}$$

Let us consider solutions for which the two branches of the spectrum coincide. Setting the expression under the radical equal to zero leads to the conditions

$$|\Delta_{k\uparrow\uparrow}| = |\Delta_{k\downarrow\downarrow}|, \qquad \Delta_{k\uparrow\uparrow}\Delta^*_{k\downarrow\uparrow} + \Delta_{k\downarrow\uparrow}\Delta^*_{k\downarrow\downarrow} = 0, \tag{8}$$

which are fulfilled if and only if the matrix $\hat{\Delta}_k\hat{\Delta}_k^*$ is proportional to the identity matrix. The coefficient of proportionality, equal to

$$|\Delta_{k\downarrow\uparrow}|^2 + |\Delta_{k\uparrow\uparrow}|^2 \equiv |\Delta_k|^2, \tag{9}$$

plays the role of the gap, since for the class of solutions under consideration the quasiparticle dispersion law has the usual form for a superconductor. As is clear from (6), the condition that both branches of the spectrum coincide is equivalent to the identical vanishing of the Green function $G_{k\uparrow}$, and hence also of the corresponding averages, i.e. $\langle a_k^+ b_k\rangle = 0$. The explicit expression for all the Green functions is found from the system (6):

$$\hat{G}_k(\omega) = \frac{1}{2\pi}\,\frac{1}{\omega^2 - \xi_k^2 - |\Delta_k|^2}\begin{pmatrix}\omega + \xi_k\\ 0\end{pmatrix},$$

$$\hat{F}_k(\omega) = \frac{1}{2\pi}\,\frac{1}{\omega^2 - \xi_k^2 - |\Delta_k|^2}\begin{pmatrix}\Delta^*_{k\uparrow\uparrow}\\ \Delta^*_{k\downarrow\uparrow}\end{pmatrix}. \tag{10}$$

and the calculation of the averages from the spectral functions leads to the system of equations determining the gap:

$$\Delta_{k\uparrow\uparrow} = \frac{1}{2V}\sum_{k'} J(\mathbf{k},\mathbf{k}')\frac{\Delta_{k'\uparrow\uparrow}}{\sqrt{\xi_{k'}^2 + |\Delta_{k'}|^2}},$$

$$\Delta_{k\downarrow\uparrow} = \frac{1}{2V}\sum_{k'} J(\mathbf{k},\mathbf{k}')\frac{\Delta_{k'\downarrow\uparrow}}{\sqrt{\xi_{k'}^2 + |\Delta_{k'}|^2}}. \tag{11}$$

We see that, in the class of solutions found, the spin conservation law is violated only in averages anomalous in the number of particles; for normal averages it is satisfied. These Green functions are asymptotically exact solutions of the problem with Hamiltonian (1), since the splitting of the system of equations was carried out asymptotically exactly. The split system (6) could have been obtained from a quadratic approximating Hamiltonian. The method of extracting from the reduced Hamiltonian the quadratic part approximating it as $V \to \infty$ is indicated in ([2,3]) and in our case leads to

$$H_a = -\frac{1}{2}\sum_{k\sigma\sigma'}\Delta_{\sigma\sigma'}(\mathbf{k})\langle a_{-k\sigma'}a_{k\sigma}\rangle^* + \sum_k \xi_k a^+_{k\sigma}a_{k\sigma}$$
$$+\frac{1}{2}\sum_{k\sigma\sigma'}\left(\Delta^*_{\sigma\sigma'}(\mathbf{k})a_{-k\sigma'}a_{k\sigma} + \Delta_{\sigma\sigma'}(\mathbf{k})a^+_{k\sigma}a^+_{-k\sigma'}\right), \tag{12}$$

where the definition of $\Delta_{\sigma\sigma'}(\mathbf{k})$ coincides with ours. But Hamiltonian (12) can be diagonalized by means of a canonical transformation of the form

$$a_{k\sigma} = u_k\alpha_{k\sigma} + \sum_{\sigma'} v_{k;\,\sigma,\sigma'}\alpha^+_{-k,\sigma'}, \tag{13}$$

which violates the spin selection rules only in quasimeans anomalous in the number of particles. Thus it is clear that one may at once put $G_{k\downarrow} = 0$, and this leads only to solutions with a single branch in the spectrum of one-particle excitations.

Let us now turn to system (11). In deriving it we nowhere used the restrictive assumption (2), so that everything said above is valid for any superposition of odd orbital angular momenta. We shall obtain the solution of the equations only for $l = 1$. For an isotropic gap the equations (11), with logarithmic accuracy, have the form (in a layer of thickness 2Λ near the Fermi sphere)

$$\Delta_{\uparrow\uparrow}(\hat{k}) = \frac{1}{4\pi}N(0)\ln\frac{2\Lambda}{|\Delta|}\int d\hat{k}'\,J(\hat{k}\cdot\hat{k}')\,\Delta_{\uparrow\uparrow}(\hat{k}'),$$
$$\Delta_{\downarrow\uparrow}(\hat{k}) = \frac{1}{4\pi}N(0)\ln\frac{2\Lambda}{|\Delta|}\int d\hat{k}'\,J(\hat{k}\cdot\hat{k}')\,\Delta_{\downarrow\uparrow}(\hat{k}'). \tag{14}$$

Here $N(0)$ is the density of states on the surface of the Fermi sphere. From (14) and (2) it follows that the functions $\Delta_{\uparrow\uparrow}(\hat{k})$ and $\Delta_{\downarrow\uparrow}(\hat{k})$ may be chosen proportional to the spherical harmonics $Y_{1,1}(\hat{k})$ and $Y_{1,0}(\hat{k})$, respectively. The coefficients of proportionality are determined from the condition $|\Delta(\hat{k})| = \text{const}$. Taking (8) into account, we obtain

$$\hat{\Delta} = \sqrt{\frac{4\pi}{3}}\,\Delta\begin{pmatrix}\sqrt{2}Y_{1,1}(\hat{k}) & Y_{1,0}(\hat{k})\\ Y_{1,0}(\hat{k}) & -\sqrt{2}Y_{1,-1}(\hat{k})\end{pmatrix}, \qquad \Delta = 2\Lambda e^{-3/gN(0)}. \tag{15}$$

It can be shown that the isotropic solution corresponds to a lower value of the energy than any anisotropic one; in particular, it is lower than for the Anderson-Morel type solution, which we obtain by putting $\Delta_{\downarrow\uparrow}(\hat{k}) = 0$. For these two solutions, the ratio of the energy of the isotropic state to that of the anisotropic one, taken in absolute value, is equal to $3\exp(-2/3) > 1$.

Let us make a few further remarks concerning the correlation functions in the model under consideration. The one-particle correlation function of the form

$$\langle\psi^+_{\sigma_1}(\mathbf{r}_1)\psi_{\sigma_2}(\mathbf{r}_2)\rangle$$

vanishes for $\sigma_1 \neq \sigma_2$ and has the same structure as in Bardeen' s model. As for the anomalous correlation function

$$\left\langle\psi_{\sigma_1}(\mathbf{r}_1)\psi_{\sigma_2}(\mathbf{r}_2)\right\rangle,$$

then, in view of the absence of spin selection rules for it, we have not one, but two essentially different functions:

$$\varphi_1(\mathbf{r}) = \frac{1}{V}\sum_k \langle b_{-k}a_k\rangle\, e^{i\mathbf{kr}}, \qquad \varphi_2(\mathbf{r}) = \frac{1}{V}\sum_k \langle a_k a_{-k}\rangle\, e^{i\mathbf{kr}}. \tag{16}$$

The function $\Phi_{\sigma_1\sigma_2}(\mathbf{r}_1 - \mathbf{r}_2)$ is antisymmetric with respect to the spatial coordinates and symmetric with respect to the spin coordinates. Thus, the wave functions of the pairs $\langle b_{-k}a_k\rangle$, $\langle a_{-k}a_k\rangle$, $\langle b_{-k}b_k\rangle$ correspond to three different orientations of the projection of the total spin on the z-axis, equal respectively to $0, 1$, and -1. We thus have a condensate formed by bound pairs in different triplet states. The number densities of pairs in these states, which we denote respectively by ρ_0, ρ_1, and ρ_{-1}, are equal to

$$\rho_1 = \rho_{-1} = \int |\varphi_2(\mathbf{r})|^2 d\mathbf{r}, \qquad \rho_0 = 2\int |\varphi_1(\mathbf{r})|^2 d\mathbf{r}, \tag{17}$$

which in the usual approximation gives the result

$$\rho_1 = \rho_{-1} = \rho_0 \simeq \frac{1}{3}\frac{\pi}{4}\, N(0)\Delta. \tag{18}$$

The pair correlation function, defined by the expression

$$\left\langle\psi^+_{\sigma_1}(\mathbf{r}_1)\psi^+_{\sigma_2}(\mathbf{r}_2)\psi_{\sigma_2'}(\mathbf{r}_2')\psi_{\sigma_1'}(\mathbf{r}_1')\right\rangle,$$

can be expressed in terms of simultaneous ones by Wick' s theorem, which is valid in this model exactly as $V \to \infty$. It is not difficult to verify that the resulting expression satisfies the principle of weakening of correlations ([2,4]).

The generalization to the case of nonzero temperature can be easily carried out by the method developed in ([3]).

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Note: Figure translations are in progress. See original paper for figures.