Pis'ma v ZhETF, vol.68, iss.6, pp.491 - 496

SUPERCONDUCTIVITY IN THE PRESENCE OF FERMION CONDENSATION

V.R.Shaginyan

St.-Petersburg Nuclear Physics Institute RAS

188350 Gatchina, Russia

Submitted 17 August 1998

Fermion condensation (FC) was studied within the density functional theory. FC can fulfill the role of a boundary, separating the region of strongly interacting electron liquid from the region of strongly correlated electron liquid. Consideration of the superconductivity in the presence of FC has shown that under certain circumstances, at temperatures above T_c the superconductivity vanishes, while the superconducting gap smoothly transforms into a pseudogap. The pseudogap occupies only the part of the Fermi surface, shrinking with increasing temperature and vanishing at $T = T^*$, while the single particle excitations of the gapped area of the Fermi surface have the width $\gamma \sim (T - T_c)$.

PACS: 71.27+a, 74.20-z

Recently a powerful method was developed for measuring the electronic structure close to the Fermi level [1]. As the result, a plateau adjacent to the Fermi level has been observed in the electronic spectra of a number strongly correlated metals. Thus, it was shown that optimally doped high temperature superconductors exhibit an anomalous normal state [1]. For instance, the spectra of Sr_2RuO_4 or $YBa_2Cu_4O_{7-\delta}$ (YBCO) contain very smooth segments on the Fermi surface. It is a remarkable thing that these spectra have not been reproduced in theoretical calculations [2]. It was shown that such peculiarities of the electronic spectra can be understood within the framework of the theory of fermion condensation (FC), which was predicted in [3] and associated with the rearrangement of the single-particle degrees of freedom in strongly correlated Fermi systems. The main feature of FC is the appearance of a plateau in the single-particle excitation spectrum at the Fermi level [3–5]. On the other hand, the quite unusual behavior in underdoped high temperature superconductors, which indicates a pseudogap above T_c, has been revealed [6–9]. As we shall see such a behavior can be also clarified within a concept of the fermion condensation.

It has been demonstrated that the onset of the density-wave instability in a Fermi system can be preceded by the FC phase transition, thus, FC can take place if the effective coupling constant is sufficiently strong [10]. This makes one think that FC is a rather widespread phenomenon inherent in strongly correlated Fermi systems. For example, FC can arise in such an unusual system as fermions locked in vortex cores in a superfluid Fermi liquid [11]. On the other hand, it was demonstrated that the charge-density wave instability takes place in three-dimensional [12] and two-dimensional electron liquid [13]. Thus, the electronic systems of some strongly correlated metals are suited for searching for FC [14].

Now let us outline the key points of the FC theory [5, 15]. FC is related to a new class of solutions of the Fermi-liquid-theory equation [16]

$$\frac{\delta(F - \mu N)}{\delta n(p,T)} = \varepsilon(p,T) - \mu(T) - T \ln \frac{1 - n(p,T)}{n(p,T)} = 0, \qquad (1)$$

for the quasiparticle distribution function $n(p,T)$, depending on the momentum p and temperature T. Here F is the free energy, μ is the chemical potential, while $\varepsilon(p,T) = = \delta E/\delta n(p,T)$ is the quasiparticle energy, being a functional of $n(p,T)$ just like the energy E and the other thermodynamic functions. Eq. (1) is usually rewritten in the form of the Fermi – Dirac distribution

$$n(p,T) = \left\{1 + \exp\left[\frac{(\varepsilon(p,T) - \mu)}{T}\right]\right\}^{-1}. \tag{2}$$

In homogeneous matter, the standard solution $n_F(p,T=0) = \theta(p_F - p)$, with p_F being the Fermi momentum, is obtained assuming that the effective mass,

$$\frac{1}{M^*} = \frac{d\varepsilon(p,T=0)}{pdp}|_{p=p_F}, \tag{3}$$

is positive and finite at the Fermi momentum p_F. As the result T-dependent corrections to M^*, quasiparticle energy, and the other quantities start with T^2-terms. But this solution of eq. (1) is not the only one. There exist "anomalous" solutions [3, 11] of eq. (1) associated with a so-called fermion condensation [3]. Being continuous within a region in p, such a solution $n(p)$ admits a finite limit for the logarithm in eq. (1) at $T \to 0$, yielding

$$\varepsilon(p) = \frac{\delta E}{\delta n(p)} = \mu, \quad p_i \le p \le p_f. \tag{4}$$

Thus, within the region $p_i < p < p_f$, the solution $n(p)$ deviates from the Fermi step function $n_F(p)$ in such a way that the energy $\varepsilon(p)$ stays constant while outside this region $n(p)$ coincides with $n_F(p)$. We see that the occupation numbers $n(p)$ become variational parameters: the solution $n(p)$ emerges if the energy E is lowered by alteration of the occupation numbers. New solutions, as it is seen from eq. (1), possess at low T the shape of the spectrum $\varepsilon(p,T)$ linear in T [14]:

$$\varepsilon(p,T) - \mu(T) \sim T << T_f, \tag{5}$$

within the interval occupied by the fermion condensate. If $T << T_f$ it follows from eqs. (1), (5) that

$$M^* \sim N(0) \sim \frac{1}{T}, \tag{6}$$

with $N(0)$ being the density of states at the Fermi level. Here T_f is the quasi-FC phase transition temperature above which FC effects become insignificant [15]. The quasiparticle formalism is applicable to this problem since the damping of the condensate states is small compared to their energy. Obviously, this condition holds for superfluid systems, while for a normal system it is also true [15].

In this Letter basing on the density functional theory the influence of FC on the superconducting phase transition is considered, including study of the pseudogap.

We start with a general consideration of the superconductivity in the presence of FC. In the density functional theory of superconductivity, there exists a unique functional $F(T)$ of two densities, namely, the normal density of an electron system ρ and the anomalous density κ. In atomic units, the functional $F[\rho,\kappa]$ is given by [17],

$$F[\rho,\kappa] = T_s[\rho,\kappa] - TS_s[\rho,\kappa] + \int \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d^3\mathbf{r}_1 d^3\mathbf{r}_2 + F_{xc}[\rho,\kappa] -$$

$$-\int \kappa^*(\mathbf{r}_1,\mathbf{r}_2)V(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)\kappa(\mathbf{r}_3,\mathbf{r}_4)d^3\mathbf{r}_1 d^3\mathbf{r}_2 d^3\mathbf{r}_3 d^3\mathbf{r}_4 = E[\rho,\kappa] - TS_s[\rho,\kappa]. \quad (7)$$

Here $T_s[\rho,\kappa]$ and $S_s[\rho,\kappa]$ stand for the kinetic energy and the entropy of a noninteracting system, while $F_{xc}[\rho(\mathbf{r}),\kappa(\mathbf{r}_1,\mathbf{r}_2)]$ is the exchange-correlation free-energy functional, V is a pairing interaction. The third and fifth terms on the r.h.s. of (7) are the Hartree terms due to the Coulomb forces and the pairing interaction, respectively. We suppose V to be sufficiently weak like the model BCS-interaction [18]. The last equality in eq. (7) can be considered as the definition of E. For the densities ρ and κ one can employ quite general forms,

$$\rho(\mathbf{r}_1) = \sum_n [|\phi_n(\mathbf{r}_1)|^2|v_n|^2(1-f_n) + |\phi_{-n}(\mathbf{r}_1)|^2|u_n|^2 f_n]; \quad (8)$$

$$\kappa(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{2}\sum_n [\phi_n^*(\mathbf{r}_1)\phi_{-n}(\mathbf{r}_2) + \phi_n^*(\mathbf{r}_2)\phi_{-n}(\mathbf{r}_1)]v_n^* u_n(1-2f_n), \quad (9)$$

with the coefficients v_n and u_n, obeying the conditions, $|v_n|^2 + |u_n|^2 = 1$. Here n denotes the quantum numbers such as the momentum p in the case of homogeneous matter or the crystal momentum and the band index in the solid state. For the sake of simplicity, we omit the spin variables. Since we are going to take a fresh look at eq. (4) we set $T = 0$. Minimization of F with respect to ϕ_n leads to the eigenfunction problem,

$$\left(-\frac{\nabla^2}{2} + \int \frac{\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|}d^3\mathbf{r}_2\right)\phi_m(\mathbf{r}_1) + \int v_{xc}(\mathbf{r}_1,\mathbf{r}_2)\phi_m(\mathbf{r}_2)d^3\mathbf{r}_2 = \varepsilon_m\phi_m(\mathbf{r}_1), \quad (10)$$

with v_{xc} being a nonlocal potential [19]. In the case of a homogeneous system the functions ϕ_m are plain waves, $|v_p|^2 = n_p$, and eq. (10) reduces to $p^2/2 + v(p) = \varepsilon(p)$. Taking into account eq. (10), one can also infer that $\delta E/\delta|v_l|^2 = \varepsilon_l$. If V were zero, ε_l would represent the real single-particle excitation spectra of system. The energy ε_l is perturbed by the BCS correlations, but, in fact, this perturbation is small. It is convenient to take $v_l = \cos\theta_l$; $u_l = \sin\theta_l$, while minimization with respect θ_l yields,

$$\frac{\delta F[\rho_1,\kappa]}{\delta\theta_l} = (\varepsilon_l - \mu)\tan 2\theta_l + \Delta_l = 0. \quad (11)$$

The gap Δ_l is given by,

$$\Delta_l = -\int \frac{\delta F[\rho_1,\kappa]}{\delta\kappa(\mathbf{r}_1,\mathbf{r}_2)}\phi_l^*(\mathbf{r}_1)\phi_{-l}(\mathbf{r}_2)d^3\mathbf{r}_1 d^3\mathbf{r}_2. \quad (12)$$

We shall now give further proof of eq. (4) deduced at $T = 0$. Consider eq. (11) in the limit $V = 0$. In this case, $\Delta_l = 0$, and eq. (11) can be written as

$$(\varepsilon_l - \mu)\tan 2\theta_l = 0. \quad (13)$$

Eq. (13) requires that,

$$\varepsilon_l - \mu = 0, \quad \text{if} \quad |v_l|^2 \neq 0, 1. \quad (14)$$

Therefore, the fermion condensation solution is a new solution of the old equations. On the other hand, it is seen from eq. (14) that the standard Kohn–Sham scheme for the single particle equations is no longer valid beyond the point of the FC phase transition, since

the quasiparticle occupation numbers $|v_l|^2$ become variational parameters, minimizing the total energy. In the homogeneous limit eq. (14) takes form of eq. (4).

FC is related to the unbounded growth of the density of states when $T \to 0$, see eq. (6). As the result, FC serves as a source for new phase transitions which lift the degeneracy of the spectrum. We are going to analyze the situation when the superconductivity wins the competition with the other phase transitions. Now let us switch on the interaction V. Then, as it follows from eqs. (7), (12), $\Delta \sim V$, when V is sufficiently small [3, 15], while in the BCS-case Δ, given by eq. (12), is exponentially small. Inserting the result $\Delta \sim V$ into eq. (7), one finds that the pairing correction $\delta E_s(T=0)$ to the ground state energy at $T=0$, $\delta E_s(T=0) \sim \Delta$[15]. This result differs drastically from the ordinary BCS result $\delta E_s \sim \Delta^2$. In response to this, an essential increase of the critical magnetic field, destroying superconductivity, can be expected. Above the critical temperature the system under consideration is in its anomalous normal state, eq. (5) is valid, and one can observe the smooth segments of the spectra at the Fermi level [9].

Now we focus our attention on an investigation of the pseudogap which is formed above T_c in underdoped high temperature superconductors [6–9]. Let us consider a 2D liquid on a simple square lattice which has a superconducting state with the d-wave symmetry of the order parameter κ. We assume that the long-range component $V_{lr}(\mathbf{q})$ of a particle-particle interaction $V_{pp}(\mathbf{q})$ is large and repulsive and has such a radius q_{lr} that $p_F/q_{lr} \sim 1$. The short-range component $V_{sr}(\mathbf{q})$ is relatively small and attractive, with its radius $p_F/q_{sr} >> 1$ [20]. As the result, the low temperature gap Δ in agreement with d-symmetry is given by [20, 21],

$$\Delta(\phi) \simeq \Delta_1 \cos 2\phi = \Delta_1 (x^2 - y^2), \tag{15}$$

with Δ_1 being the maximal gap. At finite temperatures eq. (12) for the gap can be written as,

$$\Delta(p,\phi) = -\int_0^{2\pi} V_{pp}(p,\phi,p_1,\phi_1)\kappa(p_1,\phi_1)\tanh\frac{E(p_1,\phi_1)}{2T}\frac{p_1 dp_1 d\phi_1}{4\pi^2}, \tag{16}$$

with p being the absolute value of the momentum, while ϕ is the angle. It is also suggested that FC arises near the van Hove singularities and the different areas of FC overlap slightly [14]. Because of the chosen interaction V_{pp} and then from eq. (15) it follows that Δ is to change sign,

$$\Delta(\frac{\pi}{4} + \phi) = -\Delta(\frac{\pi}{4} - \phi), \tag{17}$$

vanishing at $\pi/4$. Thus, Δ can be expanded in Taylor series around $\pi/4, p \approx p_F$:

$$\Delta(p,\theta) = a\theta - b\theta^3, \tag{18}$$

with θ being counted from $\pi/4$. Hereafter we shall consider the solutions of eq. (16) on the interval $0 < \theta < \pi/4$. Recast eq. (16), setting $p \approx p_F$ and separating out the contribution I_{lr} which comes from V_{lr}, while the contribution related to V_{sr} is denoted by I_{sr}. At small angles the contribution I_{lr} can be approximated by $I_{lr} = \theta A + \theta^3 B$. The quantities A and B are independent of T if $T \le T^* << T_f$ since they are defined by the integral running over the regions occupied by FC. This finding is consistent with the experimental results which show that Δ_1 is essentially T-independent [9]. Thus, one has

for Δ,

$$\Delta(\theta) = I_{sr} + I_{lr} = -\int_0^{2\pi} V_{sr}(\theta, p, \phi)\kappa(p, \phi) \tanh \frac{E(p, \phi)}{2T} \frac{pdpd\phi}{4\pi^2} + \theta A + \theta^3 B. \quad (19)$$

In eq. (19) the variable p was omitted. It is seen from eq. (19) that the function of FC is to produce the free term $\theta A + \theta^3 B$. We shall show that at $T \geq T_c$ the solution of eq. (19) has the second node at $\theta_c(T)$ in the vicinity of the first node $\pi/4$. To show it let us simplify eq. (19) to an algebraic equation. The quantity $I_{sr} \sim (V_0/T)\theta$ since $\tanh(E/2T) \sim E/2T$ if $T \approx T_c$, while $V_0 \sim V_{sr}$ is a constant. Upon dividing both part of eq. (19) on $\kappa(\theta)$, one gets,

$$E(\theta) = -(\frac{V_0}{T} - A_1 - \theta^2 B_1)|\theta|, \quad (20)$$

with A_1, B_1 being new constants. The quantity A_1 is negative and it is inferred from the condition that eq. (16) has the only solution $\Delta \equiv 0$ when $V_{sr} = 0$, while B_1 is positive. The factor in brackets on the r.h.s. of eq. (20) changes its sign at some temperature $T = T_c \approx V_0/A_1$, on the other hand, the excitation energy must be $E(\theta) > 0$, as the result the gap has to reverse its sign on the interval Ω $[0 < \theta < \theta_c]$, with $\Delta(\theta_c) = \Delta(0) = 0$. It is seen from eq. (20) that the angle θ_c is related to $T > T_c$ by the equation,

$$T \approx \frac{V_0}{(A_1 + B_1\theta_c^2)}. \quad (21)$$

Our estimations of the maximal gap Δ_0 in the range Ω show that $\Delta_0 \sim 10^{-3}\Delta_1$. Thus we can conclude that the gap in the range Ω can be destroyed by strong antiferromagnetic correlations which exists in underdoped superconductors [22, 23]. Then, it is believed that impurities can easily destroy Δ in the considered area. Now one can conclude from eq. (20) that T_c is the temperature when the superconductivity vanishes, while the gap, which is also referred to as a pseudogap, persists outside the region. It is seen from eq. (21) that $\theta_c \sim \sqrt{(T - T_c)/T_c}$, thus one can expect that the pseudogap dies out as a temperature T^* is approached.

Now consider the quasiparticle excitations at the Fermi level. At temperatures $T < T_c$ they are typical excitations of the superconducting state. At $T > T_c$ in the range Ω we have normal quasiparticle excitations with a width γ. The other part of the Fermi level is occupied by the BCS like excitations with the finite energy of excitation, given by the gap $\Delta(\phi)$, while both type of the excitations have the widths of the same order of magnitude. Let us estimate γ. If the entire Fermi level were occupied by the normal state the width would be equal, $\gamma \sim N(0)^3T^2/\alpha^2$, with the density of states $N(0) \sim 1/T$, and the dielectric constant $\alpha \sim N(0)$. Thus one has, $\gamma \sim T$ [15]. But in our case only part of the Fermi level within Ω belongs to the normal excitations. Therefore, the number of states allowed for quasiparticles and for quasiholes are proportional to θ_c, and thus the factor T^2 is replaced by $T^2\theta_c^2$. Having regard to these factors, one gets, $\gamma \sim \theta_c^2 T \sim T(T - T_c)/T_c \sim (T - T_c)$ since we consider only small angles. Here we have omitted the small contribution coming from the BCS like excitations, that is why the width γ vanishes at $T = T_c$. Thus, we can conclude that above T_c the superconducting gap smoothly transforms into the pseudogap. The excitations of the gapped area of the Fermi surface have the same width $\gamma \sim (T - T_c)$, and the region occupied by the pseudogap

is shrinking with increasing temperature. These results are in good agreement with the experimental facts [6–9].

A few remarks are in order at this point. Basing on the previous consideration, we can conclude that BCS-type approach is fruitful for consideration of underdoped samples. It is worth noting that Δ_1 scales with T^* rather then with T_c [7], since T^* defines the existence of non-trivial solutions of eq. (16), while T_c is related to the emergence of the new nodes of the gap. Then, the peak was observed in inelastic neutron scattering from single crystals of optimally doped YBCO and of underdoped samples, at temperatures below T_c, while the broad maximum above T_c exists in underdoped samples [21]. The explanation of this peak, based on the ideas of the BCS theory, was given in [24]. One can recognize that the same explanation holds for the broad maximum in underdoped samples above T_c.

In summary, we have considered FC within the density functional theory. The FC phase transition manifests itself when the effective coupling constant is sufficiently large. FC can fulfill the role of a boundary, separating the region of strongly interacting electron liquid from the region of strongly correlated electron liquid. We have also considered the superconductivity in the presence of FC. As the result, we were led to the conclusion that under certain circumstances, at temperatures above T_c, the superconducting gap smoothly transforms into a pseudogap. The pseudogap occupies only the part of the Fermi surface, shrinking with increasing temperature and vanishing at $T = T^*$, while the single particle excitations of the gapped area of the Fermi surface have the width $\gamma \sim (T - T_c)$.

This research was funded in part by the Russian Foundation for Basic Research under Grant 98-02-16170. The work has benefited from discussions with V. Belincher, M. de Llano, V.A. Khodel, and G.E. Volovik.

---

1. Z.-X.Shen and D.S.Dessau, Phys. Rep. **253**, 1 (1995).
2. D.J.Singh, Phys. Rev. **B54**, 13311 (1996).
3. V.A.Khodel and V.R.Shaginyan, JETP Lett. **51**, 553 (1990).
4. G.E.Volovik, JETP Lett. **53**, 208 (1991).
5. V.A.Khodel, V.R.Shaginyan, and V.V.Khodel, Phys. Rep. **249**, 1 (1994).
6. H.Ding et al., Nature **382**, 51 (1996).
7. H.Ding et al., cond-mat/9712100 9 Dec. 1997.
8. M.R.Norman et al., cond-mat/9710163 15 Oct. 1997.
9. M.R.Norman et al., cond-mat/9711232 21 Nov. 1997.
10. V.A.Khodel, V.R.Shaginyan, and M.V.Zverev, JETP Lett. **65**, 253 (1997).
11. G.E.Volovik, JETP Lett. **63**, 763 (1996).
12. M.Levy and J.P.Perdew, Phys. Rev. **48**, 11638 (1993).
13. L.Świerkowski, D.Neilson, and J.Szymański, Phys. Rev. Lett. **67**, 240 (1991).
14. V.A.Khodel, J.W.Clark, and V.R.Shaginyan, Solid St. Comm. **96**, 353 (1995).
15. J.Dukelsky, V.A.Khodel, P.Schuck, and V.R.Shaginyan, Z. Phys. **102**, 245 (1997).
16. L.D.Landau, JETP **30**, 1058 (1956).
17. L.N.Oliveira, E.K.U.Gross, and W.Kohn, Phys. Rev. Lett. **60**, 2430 (1988).
18. J.Bardeen, L.N.Cooper, and J.R.Schrieffer, Phys. Rev. **108**, 1175 (1957).
19. V.R.Shaginyan, Proceedings of CMT22, in press (1997).
20. D.J.Scalapino et al., Phys. Rev. **B34**, 8190 (1986); D.J.Scalapino, Phys. Rep. **250**, 329 (1995).
21. A.A.Abrikosov, Physica **C222**, 191 (1994).
22. J.Schmalian, D.Pines, and B.Stojkovic, Phys. Rev. Lett. **80**, 3839 (1998).
23. I.A.Privorotsky, JETP **43**, 2255 (1962).
24. A.A.Abrikosov, Phys. Rev **B57**, 8656 (1998).