

Influence of correlated impurities on the onset of Cooper pairing

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Effect of two-particle correlations between impurities on the temperature of transition of a Fermi liquid in the superfluid or superconducting state is analyzed. It is shown, that correlations with a radius, exceeding correlation length of the superconductor can have a pronounced effect on the transition temperature. The equation for the transition temperature is corrected for correlations of the impurities. Possible applications of the new equation are discussed.

1. Effect of impurities or vacancies on thermodynamic properties of traditional superconductors is well described by the Abrikosov and Gorkov (AG in what follows) theory of superconducting alloys [1]. Possible correlations among the impurities are neglected in this theory. Difference with respect to the pure superconductor in this theory is characterized by one parameter – electron mean free path l relative to the coherence length of the superconductor ξ_0 . It has been observed recently [2] (and references therein), that certain impurities in the high- T_c compounds demonstrate a tendency to short-range ordering, which influences the superconducting transition temperature T_c of the compound. Even more clear example of such influence is presented by the superfluid ^3He in a high-porosity aerogel [3, 4]. Aerogel is a rigid structure consisting of strands of a diameter $a \approx 3\text{ nm}$ and the average distance between the strands $\xi_a \approx 40\text{ nm}$ for 98% porosity. The latter distance is usually taken as a characteristics of correlations within aerogel. Thermodynamic properties of ^3He in aerogel, in particular dependence of the suppression of the transition temperature with respect to that of pure ^3He on ξ_0/l demonstrate significant deviation from the universal behavior, predicted by AG-theory. This deviation was attributed to the existence of structural correlations in aerogel with a correlation radius which is comparable with ξ_0 [5]. In 98% aerogel depending on a pressure ξ_0 for ^3He varies from infinity at $P \approx 5\text{ bar}$ to $\xi_0 \approx 20\text{ nm}$ at solidification. The condition $\xi_a \approx \xi_0$ is met at $P \approx 15\text{ bar}$.

In the present paper effect of correlations on T_c is considered under assumption that the correlations are weak. Parameter, which characterizes deviation from the AG-theory turns out to be the ratio $R^2/\xi_0 l_{tr}$, where R is a length, characterizing correlation of impurities. For aerogel $R \sim \xi_a$ and the effect of correlations on the T_c can be significant. Analogous approach was used before for the situation when suppression of T_c is small in comparison with the original T_c [6]. Here this restriction

is lifted and the argument is extended for arbitrary suppression of T_c . This generalization is necessary for ^3He in aerogel since at a pressure about 6 bar the observed T_c is zero so that the suppression of T_c is equal to T_c itself.

2. Transition temperature T_c is defined as a temperature of the onset of the long-range order. At this temperature appears a pole in the thermodynamic vertex part $\Gamma(\Omega_n, \mathbf{q})$ for scattering of two quasi-particles with the total momentum $\mathbf{q} = 0$ and the total frequency $\Omega_n = 0$ [7]. Equation for T_c has the standard form for all types of Cooper pairing:

$$1/\lambda = \Pi(0, 0), \quad (1)$$

where λ is a constant of the pairing interaction and polarization operator is defined as

$$\begin{aligned} \Pi(\mathbf{q}, \Omega_n) &= \\ &= T \sum_m \int \frac{d^3k}{(2\pi)^3} G(\mathbf{k} + \mathbf{q}, \omega_m + \Omega_n) G(-\mathbf{k}, \omega_{-m}) \equiv \\ &\equiv T \sum_m L_m^{(0)}(\mathbf{q}, \Omega_n), \end{aligned} \quad (2)$$

$G(\mathbf{k}, \omega_n)$ etc. are thermodynamic Green functions of quasi-particles. In what follows $L_m^{(0)}(\mathbf{q}, \Omega_n)$ always enters at $\Omega_n = 0$, and a shorthand notation $L_m^{(0)}(\mathbf{q}, 0) \equiv \equiv t_m(\mathbf{q})$ is used.

Effect of impurities is described by the potential

$$U(\mathbf{r}) = \sum_a u(\mathbf{r} - \mathbf{r}_a) \quad (3)$$

which is a sum of individual potentials of impurities, situated in positions \mathbf{r}_a . These positions are random. In the standard technique [7] the Green functions of quasi-particles are expanded in the Born series over $U(\mathbf{r})$ and averaged over positions of the impurities. The sum of the obtained series can be written as:

$$\langle G(\varepsilon; \mathbf{k}, \mathbf{k}') \rangle = 2\pi\delta(\mathbf{k} - \mathbf{k}') [G_0^{-1} - \langle \Sigma \rangle]^{-1}, \quad (4)$$

where $\langle \Sigma \rangle$ is the averaged self-energy. Two first terms of the Born series for $\langle \Sigma \rangle$ are represented by the dia-

grams Fig.1. Correlations among the impurities introduce changes in the procedure of averaging.

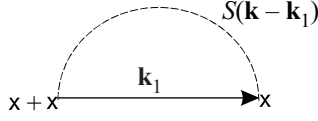


Fig.1

To every cross corresponds a function $u(\mathbf{k}' - \mathbf{k}) \sum_a e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}_a}$, where \mathbf{k} and \mathbf{k}' – the incoming and out-going momenta. Essential contribution comes from the term with two crosses. It is proportional to the averaged sum: $\langle \sum_{a,b} e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}_a + i(\mathbf{k}_1-\mathbf{k}')\mathbf{r}_b} \rangle$. Summation over \mathbf{r}_a renders a factor $(2\pi)^3 n \delta(\mathbf{k} - \mathbf{k}')$. The remaining sum is a structure factor

$$S(\mathbf{q}) \equiv \langle \sum_b e^{i\mathbf{q}(\mathbf{r}_b - \mathbf{r}_a)} \rangle, \quad (5)$$

where $\mathbf{q} = \mathbf{k}_1 - \mathbf{k}$. For uncorrelated impurities $S(\mathbf{q}) = 1 + (2\pi)^3 n \delta(\mathbf{q})$. The unity comes from the summand with $\mathbf{r}_b = \mathbf{r}_a$. The term with $\delta(\mathbf{q})$ can be dropped, because in further calculations it enters with the factor $u(0)$, which is excluded by a shift of the ground state energy. When correlations are present there appears an additional term $\bar{S}(\mathbf{q})$ which is directly related to the correlation function in the coordinate representation. Summation in Eq.(5) for $\mathbf{r}_b \neq \mathbf{r}_a$ can be changed for integration with the probability $w(\mathbf{r}_b|\mathbf{r}_a)$ to find a particle in the point \mathbf{r}_b if there is a particle in the point \mathbf{r}_a . In the isotropic case $w(\mathbf{r}_b|\mathbf{r}_a)$ depends on a relative distance $r = |\mathbf{r}_b - \mathbf{r}_a|$. At $r \rightarrow \infty$ correlations vanish and $w(r)$ tends to a constant. Normalization of $w(r)$ is chosen so that this constant is unity. A measure of correlations is $v(r) = w(r) - 1$ (cf. [8]). With these notations

$$\bar{S}(\mathbf{q}) = n \int v(r) e^{-i\mathbf{q}\mathbf{r}} d^3r \quad (6)$$

and

$$\Sigma_2(\varepsilon; \mathbf{k}) =$$

$$= n \int u(\mathbf{k}_1 - \mathbf{k}) u(\mathbf{k} - \mathbf{k}_1) [1 + \bar{S}(\mathbf{k} - \mathbf{k}_1)] G(\varepsilon; \mathbf{k}_1) \frac{d^3k_1}{(2\pi)^3}. \quad (7)$$

Integration of two crosses in one block Σ_2 is graphically represented by the dashed line, connecting the crosses (cf. Fig.1). To this line corresponds now the sum $1 + \bar{S}(\mathbf{q})$. The averaged Green function has the same form as for uncorrelated impurities

$$\langle G(\omega_n; \mathbf{k}, \mathbf{k}') \rangle = (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}') (i\omega_n - \mu + \frac{i}{2\tau} \text{sgn}\omega_n)^{-1}, \quad (8)$$

except that the average inverse time between the collisions includes $\bar{S}(\mathbf{q})$:

$$\frac{1}{\tau} = 2\pi n \nu_0 \int |u(\theta)|^2 [1 + \bar{S}(\theta)] \frac{d\Omega}{4\pi}. \quad (9)$$

Here θ is the angle between \mathbf{k}_1 and \mathbf{k} . The new term $\bar{S}(\theta)$ takes into account effect of interference of de Broigle waves of quasiparticles scattered by different impurities. This effect can be formally included in the definition of cross-section $|\overline{u(\theta)}|^2 = |u(\theta)|^2 [1 + \bar{S}(\theta)]$. It is determined by the properties of the normal phase and does not depend on T_c . The effect of interference is usually small, since the average distance between the impurities a is large in comparison with the wave length of quasiparticles, and $\bar{S}(\mathbf{q})$ vanishes at $|\mathbf{q}| > 1/a$. Contribution of $\bar{S}(\mathbf{q})$ to the integrand in Eq. (7) is comparable with unity only at angles $\theta \sim 1/ak_F$. For small concentration of impurities x the relative contribution of correlations is on the order of $x^{2/3}$.

At the averaging of the polarization operator except for substitution of the averaged Green functions in Eq.(2) it is necessary to take into account the contribution of “ladder” diagrams of the type represented by the first diagram in the r.h.s. of the equation Fig.3. The dashed lines bring in the factor $1 + \bar{S}(\mathbf{k} - \mathbf{k}_1)$, which can also be included in the cross-section $|\overline{u(\mathbf{k}_1 - \mathbf{k})}|^2$. For definiteness the explicit analysis here is made for the p-wave pairing. That makes possible to apply the obtained results to the superfluid ^3He in aerogel. The interaction leading to the p-wave pairing is proportional to the scalar product of unit vectors $\hat{\mathbf{k}}, \hat{\mathbf{k}}'$: $V(\mathbf{k}, \mathbf{k}') = 3V_1(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}')$. As the result the loops on the left and the right ends of the ladder diagrams acquire factors $\hat{\mathbf{k}}$ and $\hat{\mathbf{k}}'$ respectively. The cross-section of scattering on the spherically symmetric impurities can be expanded in a series of Legendre polynomials:

$$|\overline{u(\mathbf{k}_1 - \mathbf{k})}|^2 = \sigma_0 + 3\sigma_1(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}') + 5\sigma_2 P_2(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}') + \dots \quad (10)$$

After the angular integration in every loop of the ladder diagrams only σ_1 -component remains. It enters results via inverse collision time $1/\tau_1 = 2\pi\nu_0\sigma_1$. Summation of the series for $\Pi(0, 0)$ renders familiar equation for T_c at the p-wave Cooper pairing:

$$1 = 2\pi\nu_0 V_1 \sum_{n \geq 0} \frac{1}{\omega_n + 1/2\tau_{tr}}, \quad (11)$$

where $1/\tau_{tr} = 2\pi n \nu_0 (\sigma_0 - \sigma_1)$. For the pairing with other angular momenta $l \neq 1$ a proper σ_l and $1/\tau_l$ have to be used. In particular for the case of s-wave pairing the resulting $1/\tau$ would be zero and transition temperature is not lowered in agreement with Refs. [1, 9].

So, within the scheme of the AG theory, correlations among the impurities enter the equation for T_c only im-

PLICITLY, via the mean free path, determined by the normal phase.

3. A non-trivial effect of correlations occurs when the contribution of diagrams with four crosses is taken into account in $\Pi(\mathbf{q}, \Omega_n)$. Of particular interest for the present discussion are the diagrams with three dashed lines as shown on the Fig.2.

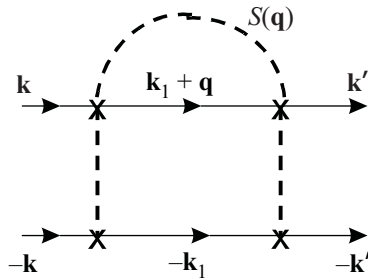


Fig.2

Without correlations it would correspond to the fourth order correction to the amplitude of scattering of two quasiparticles with zero total momentum on the same impurity. For interacting quasiparticles in the intermediate state instead of the product of two single particle Green functions $G_n(\mathbf{k}_1 + \mathbf{q}_1)G_{-n}(-\mathbf{k}_1)$ the two-particle Green function $G^{II}(\mathbf{k}_1 + \mathbf{q}_1, -\mathbf{k}_1, \omega_l, -\omega_l; \mathbf{k}_2 + \mathbf{q}_1, -\mathbf{k}_2, \omega_m, -\omega_m)$ has to be used. As a function of \mathbf{q}_1 G^{II} is singular at $\mathbf{q}_1 = 0$. This singularity corresponds to formation of a virtual Cooper pair. It increases the weight of states with $\mathbf{q}_1 \sim 1/\xi_0$ in the integral, corresponding to this diagram. If the impurities are correlated on a distance $\sim \xi_0$ there remains a net effect of interference of the waves with $\mathbf{q}_1 \sim 1/\xi_0$ scattered by impurities. Depending on a sign of correlations it can decrease or increase the destructive effect of impurities. The aim of the following discussion is to find out when the effect of interference is essential.

Interaction of electrons conserves the total momentum \mathbf{q}_1 and the total frequency $\Omega = 0$ but, unlike the elastic scattering by impurities, it does not conserve each of the frequencies ω_l . As the result the polarization operator became a sum over two indices: $\Pi(0) = T^2 \sum_{lm} L_{lm}(0)$, where $L_{lm}(0)$ is a block, represented by the black rectangle in the Fig.3.

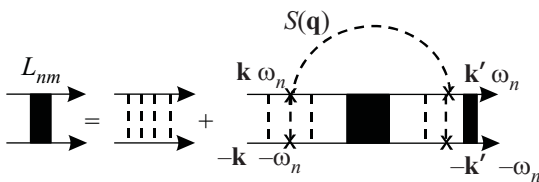


Fig.3

In analytic form the equation Fig.3 can be written as:

$$\bar{L}_m = t_m(0) - t_m(0)T \sum_j M_{mj} \bar{L}_j, \quad (12)$$

where

$$M_{mj} = n\sigma_1^2 \int t_m(\mathbf{q})\Gamma(\mathbf{q})[1 + \bar{S}(\mathbf{q})]t_j(\mathbf{q}) \frac{d^3q}{(2\pi)^3}, \quad (13)$$

$\bar{L}_j = T \sum_m L_{jm}(0)$ and $t_j(\mathbf{q}) = B_j(\mathbf{q})/[1 - n\sigma_1 B_j(\mathbf{q})]$ with $B_j(\mathbf{q}) = \frac{2\pi\nu_0}{vq} \arctg\left(\frac{vq}{2|\tilde{\omega}_j|}\right)$. In a limit $q \rightarrow 0$ it tends to $t_j(0) = 2\pi\nu_0/|\tilde{\omega}_j|$ with $\tilde{\omega}_j = \omega_j + 1/2\tau_{tr}$.

The matrix M_{mj} is proportional to σ_1^2 , which brings in a small factor $(\xi_0/l_{tr})^2$. A special situation arises when the impurities are correlated on a distance R which is greater than ξ_0 . In this case $\bar{S}(\mathbf{q})$ is enhanced in a region $q \sim 1/R$. In the limiting case $R \gg \xi_0$ all functions under the integral in Eq.(13) except for $\bar{S}(\mathbf{q})$ and $\Gamma(\mathbf{q})$ can be taken at $q = 0$ so that $M_{mj} = n\sigma_1^2 t_m(0)Q t_j(0)$, where $Q = \int \Gamma(\mathbf{q})\bar{S}(\mathbf{q}) \frac{d^3q}{(2\pi)^3}$. At the transition temperature and at small q $\Gamma(\mathbf{q}) = -\gamma/\nu_0(\xi_0 q)^2$ with coefficient $\gamma = 12/7\zeta(3)$. A singular behavior of $\Gamma(\mathbf{q})$ at $q \rightarrow 0$ increases the weight of small q in the integral and since $\bar{S}(\mathbf{q})$ is enhanced at $q \sim 1/R$ the value of the integral is also enhanced. For estimation of integrals, containing \bar{S} the form $\bar{S}(\mathbf{q}) = A\delta(q - q_0)$ with $q_0 = 1/R$ is convenient. The coefficient A is determined from the normalization condition $\int \bar{S}(\mathbf{q})d^3q = (2\pi)^3 n\nu(0)$, so that $A = 2\pi^2 R^2 n\nu(0)$. Omitting insignificant coefficients of the order of unity we arrive at

$$Q \sim -\frac{R^2}{\xi_0^2} \frac{n\nu(0)}{\nu_0(2\pi)^2}. \quad (14)$$

This estimation shows, that the second term in the rhs of Eq.(12) relative to the first is on the order of $(R/l)^2$. At $R \ll l$ Eq.(12) can be solved by iterations. As a first iteration we have:

$$\bar{L}_m = t_m(0) - t_m(0)T \sum_j M_{mj} t_j(0), \quad (15)$$

Summation of this equation over m with account of Eq.(1) after standard transformations renders the equation for T_c :

$$\ln \frac{T_c}{T_{AG}} = \psi\left(\frac{1}{2} + \frac{1}{4\pi T_{AG} \tau_{tr}}\right) - \psi\left(\frac{1}{2} + \frac{1}{4\pi T_c \tau_{tr}}\right) - f(T_c), \quad (16)$$

where

$$f(T_c) = n \frac{\sigma_1^2}{\nu_0} \int \left[T \sum_m t_m(0) t_m(\mathbf{q}) \right]^2 \Gamma(\mathbf{q}) [1 + \bar{S}(\mathbf{q})] \frac{d^3q}{(2\pi)^3} \quad (17)$$

and $\psi(z) = \frac{d}{dz} \ln \Gamma(z)$ is di-gamma function. Equations (16) and (17) form a closed system, which for given material parameters and a given form of the structure

factor determines the transition temperature in a liquid with correlated impurities. Difference with respect to the standard result T_{AG} is represented by the function $f(T_c)$ in the r.h.s. of Eq.(16).

Further iterations of Eq. (12) render consecutive terms in the expansion of the solution of Eq. (12) in powers of the parameter $(R/l)^2$. The accuracy of Eq. (12) itself is limited by a different parameter. The kernel (13) takes into account interaction of the virtual Cooper pair only with two correlated impurities. Averaging of diagrams including interaction with three correlated impurities requires knowledge of the three-particle correlation function. For estimation of the contribution of this process we can decouple the three particle correlation function in a product of the two-particle correlation functions and keep only the most singular terms. The correction would contain extra factor $Q\xi_0/l_{tr} \sim R^2/\xi_0 l_{tr}$. Higher order correlations can be neglected if this parameter is small.

For unconventional superconductors the actual situation is $\xi_0 < l_{tr}$. We assume that the strong inequality $\xi_0 \ll l_{tr}$ is met. Then there exist a window $\xi_0 \ll R \ll l_{tr}$. In a limit $R \gg \xi_0$ the asymptotic expression for $f(T_a)$ at $(R/\xi_0) \rightarrow \infty$ can be used. The function $t_m(\mathbf{q})$ in the integrand of Eq. (17) can be taken at $\mathbf{q} = 0$ and the sum over m can be done explicitly

$$T \sum_m t_m^2(0) = \frac{v_0^2}{2T} \psi' \left(\frac{1}{2} + \frac{1}{4\pi T_c \tau_{tr}} \right) \quad (18)$$

The remaining integral over \mathbf{q} in the limit $R \gg \xi_0$ is proportional to $(R/2l_1)^2$ with a coefficient $\alpha \sim 1$ depending on the explicit form of the structure factor. The resulting form of $f(T_c)$ is then:

$$f(T_a) = -\alpha \left[\frac{R}{2l_1} \psi' \left(\frac{1}{2} + \frac{1}{4\pi T_c \tau_{tr}} \right) \right]^2. \quad (19)$$

The sign of α depends on a limiting value of the correlation function $v(r)$ at $r \rightarrow 0$. At $v(0) = 0$ $\alpha < 0$, i.e. a tendency of impurities to form groups favors formation of Cooper pairs and increases T_c and vice versa.

4. For application of the obtained formulae to aerogel we have to substitute its structure factor in the definition of Q . 98% Aerogel within the interval of distances $a \ll r \ll R$ has a fractal structure with the dimensionality $D = 1.6 \div 1.8$ [5]. Its structure factor within $1/R \ll q \ll 1/a$ varies as q^{-D} . As a consequence the integral $Q \sim \int dq/q^D$ is dominated by the lower limit $\sim 1/R$. Unfortunately, the available data for the structure factor are given in arbitrary units so that the value of Q can be found only up to unknown factor. Instead of the measured structure factor a model expression was suggested [6], assuming that at $r > R$ correlations decay as $\exp(-r/R)$ R in this model is a fitting parameter.

Simplified analysis, using the limiting expression valid for $R \gg \xi_0$ can be used only at pressures above 20 bar. In this region Eqns. (16), (19) reproduce qualitative features of the experimentally observed dependence of T_c on pressure. In particular the difference $T_c - T_{AG}$ is practically constant within this interval, but the interval itself is not large enough for making definitive statements. In a region $P < 20$ bar the limiting expression for $t_m(0)$ is not sufficiently accurate and Eqns. (16),(17) have to be solved with the full $t_m(\mathbf{q})$. That requires rather involved numerical calculations which are not done yet.

In conclusion, it is shown that effect of correlations on the suppression of the transition temperature of a Fermi liquid in the superfluid (superconducting) state by impurities can be essential if correlation radius R of impurities is greater than the correlation length of a superconductor ξ_0 . Correlations can increase the transition temperature with respect to the value, given by the standard theory of superconducting alloys. The obtained equations express the transition temperature in terms of the structure factor of ensemble of impurities. The quantitative analysis takes into account only two-particle correlations. Within this approximation a relative change of T_c is characterized by the parameter $R^2/\xi_0 l_{tr}$. This parameter simultaneously determines accuracy of the approximation. If $R^2/\xi_0 l_{tr} \sim 1$, the results can be used only for qualitative estimations. Good candidates for observation of the discussed effect are superconductors with small values of ξ_0 .

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1. A. A. Abrikosov and L.P. Gorkov, ZhETF **39**, 1781 (1961), [Sov. Phys. JETP **12**, 1243 (1961)].
2. M. Fratini, N. Poccia, A. Ricci et al., Nature, **466**, 841 (2010).
3. J. V. Porto and J. M. Parpia, Phys. Rev. Lett. **74**, 4667 (1995).
4. D. T. Sprague, T. M. Haard, J. B. Kycia et al., Phys. Rev. Lett. **75**, 661 (1995).
5. J. V. Porto and J. M. Parpia, Phys. Rev. B **59**, 14583 (1999).
6. I. A. Fomin, JETP Letters **88**, 59 (2008).
7. A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzaloshinskii, *Metody kvantovoi teorii polja v statisticheskoi fizike*, M.: Nauka, 1962, Ch. VII.
8. L. D. Landau and E. M. Lifshitz, *Statistical physics*, part 1. ch. 12, - M.: Nauka, 1995.
9. P.W. Anderson, Journ. Phys. Chem. of Sol. **11**, 26 (1959).