Singular Fermi liquid as a model of unconventional superconductivity: thermodynamic and magnetic properties

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Abstract. Superconductivity in the system of strongly correlated to electrons treated as a singular Fermi liquid (SFL) is studied. In the system the scattering amplitude for particles with the same momenta is divergent. Thermodynamics of the system is discussed within the Bogolubov method. The gap equation and the equation for the chemical potential are solved. It is found that the energy gap and the chemical potential are doubly-valued in the subcritical region, however only the upper branches are thermodynamically stable. The obtained results prove that the SFL system displays some features of the superconducting state also in the supercritical temperature range. It is proposed to relate the observed phenomena to the emergence of the pseudogap. The phase transition to the superconducting state is found to be of the first order with a pronounced discontinuity in the entropy. The supercritical temperature range is considered in detail. Some of the magnetic field induced effects are also discussed: the critical magnetic field and the magnetic field penetration depth are found. Possibilities to generalize the presented results are also pointed out.

1. Introduction

Since the discovery of high-\( T_c \) superconductors (HTSC) over twenty years ago much effort has been put into explanation of their phase diagram. Sophisticated experimental methods – in particular in the area of HTSC spectroscopy [1] – revealed a fine structure of the phase diagram, especially in the case of systems near to the optimal doping. In this area of the phase diagram many anomalies have been found [2] pointing to the fact that the normal phase of HTSC should not be treated as a conventional Fermi liquid, but rather as a more complex kind of a quantum liquid (cf. [3] and references therein). The richness of the phase diagram has pushed research on the theoretical front to go beyond the limits set by the theory of Bardeen, Cooper and Schrieffer (BCS). A number of non-Fermi or singular Fermi liquid models have been proposed to deal with the anomalies observed experimentally in nearly optimally doped structures [3]. These include models with additional non-standard terms introduced into standard Hamiltonians [4-6] in order to grasp the essential properties of the HTSC. In the present paper we follow one of these paths and consider a model of a singular Fermi liquid with divergent scattering amplitude for particles with the same momenta, widely discussed in the literature [4-6].
2. Model and method

Our starting point is the effective SFL Hamiltonian, established in Refs. [4-8], with the dispersion relation $k \varepsilon_k$ (obtained e.g. from the 2D tight-binding band model), a separable pairing potential $\zeta \eta k k k k$ and the interaction $R_k n_k n_k$, responsible for scattering of particles with the same momenta $k$ and opposite spins. The scattering interaction can be separated into regular and singular parts and it is assumed that the effects of particles interaction due to the regular part, which renormalize the one-particle dispersion relation by means of the mass operator, have been included by a particular choice of the dispersion relation [9].

For an arbitrary value of the scattering amplitude $R_k$, Hamiltonian (1) acts in a 16-dimensional Fock space spanned upon the basis

$$\psi_{\sigma\sigma'}(k) = \left| k, \sigma \right\rangle \left\langle -k, \sigma' \right|,$$

with $\sigma, \sigma' = 0, \uparrow, \downarrow$ or $\uparrow\downarrow$ denoting the spin projection. However, when the scattering amplitude becomes divergent ($R_k \to \infty$), the contribution of terms corresponding to the doubly occupied states $\psi_{\sigma\sigma'}(k)$ and $\psi_{\sigma\sigma'}(k)$ to the Hamiltonian is infinitely large. Hence, these terms become energetically forbidden and the Fock space effectively reduces to a 9-dimensional one with the basis $\psi_{\sigma\sigma'}(k)$, where $\sigma, \sigma' = 0, \uparrow, \downarrow$ [7,8,12]. Consequently the SFL Hamiltonian acting in the reduced, 9-dimensional space reads

$$H_{SFL} = \sum_k \varepsilon_k (n_k \uparrow + n_k \downarrow) - \eta \sum_k \zeta \eta k k k k k k k k$$

with $\xi_k = \varepsilon_k - \mu$ and $\mu$ denotes the chemical potential.

The problem of superconductivity in the SFL characterized by the Hamiltonian (1) can be studied in a systematic manner within the Bogolubov method [10]. The main idea is to introduce the approximating Hamiltonian

$$H_{SFL}^0 = \sum_k \varepsilon_k (n_k \uparrow + n_k \downarrow + n_k \downarrow + n_k \uparrow) - \Delta_k \left( a_k \uparrow a_k \downarrow + a_k \downarrow a_k \uparrow \right) + H.c. \right\rangle$$

where the order parameter $\Delta_k$ is taken in a self-consistent manner and the (primed) sum over the momentum runs over a half of the reciprocal space only. In the next step the partition function and the corresponding thermodynamic potential are found for the approximating Hamiltonian (2) [9,11,12]. The Bogolubov method ensures that in the thermodynamic limit, the thermodynamic potential of the approximating Hamiltonian (2) converges to the thermodynamic potential of the original SFL Hamiltonian (1). The advantage of the method is that the calculations can be done in a quite general form and the results can be easily extended, e.g. including the effects of external fields or composed dispersion relations [7,11,13].

Although it is possible to consider a very general case [7,8], in order to present some crucial features of the model, the results presented and discussed in this paper have been obtained for the isotropic $s$-wave paired SFL with $\varepsilon_k = \xi_v (k - k_F)$, $\eta \zeta \xi_k = \lambda$, and $\Delta_k = \Delta(T)$. The pairing interaction has been assumed to cover the whole nearly half-filled conduction band of the width $2\omega$ [7,8,11-14].
3. Thermodynamics of the superconducting phase transition

The thermodynamics of the system is fully contained in the thermodynamic potential $\Omega$, which is given by the Bogolubov method [7,8,10]. The thermodynamic potential is related to the free energy of the system by the equation $F = \Omega + \mu N$. At non-zero temperature the stable equilibrium state of the system is determined by the usual equilibrium conditions, which require the free energy to be minimal. In the superconducting phase, the free energy of the SFL is a function of the order parameter and the chemical potential. Consequently, the equilibrium conditions imposed on the free energy yield the gap equation and the equation for the chemical potential, whose solutions provide the temperature dependence of these two quantities. Once the temperature dependence is known, one can find the temperature dependence of the free energy and other thermodynamic characteristics, such as the entropy $S(T) = -dF(T)/dT$ and the specific heat $C(T) = -T d^2F(T)/dT^2$. The same arguments apply to the normal phase, the only difference being the absence of the superconducting order parameter ($\Delta_k = 0$).

The two fundamentals equation have been solved numerically for the $s$-wave paired SFL [7,8,12] and the results are presented in Figure 1a. The striking feature of these solutions is the appearance of two branches of solutions above a certain temperature, which we will denote as $T_0$. This is in apparent contrast with the usual BCS shape of the order parameter amplitude $\Delta(T)$, cf. Figure 1b. Therefore, the temperature range $T_0 \leq T \leq T^*$, where $T^*$ denotes the highest temperature at which a solution of these two equation exists, has to be discussed in detail.

![Figure 1. Solutions of the gap equation and the equation for the chemical potential (inset) in the case of (a) SFL, (b) standard BCS system. The bandwidth $\omega / \Delta(0) = 2$ (solid), $2 / \sqrt{5}$ (dash), $10$ (dot). For details see Ref. [7].](image)

In order to decide which of the two branches of the solutions is thermodynamically stable, one can use the free energy criterion, i.e. compare the free energies of the two branches [7,8,12,14]. Then the branch of the lower free energy is the ‘physical’ one. Moreover, if its free energy is lower than the free energy of the normal phase, the SFL is in the superconducting phase. The temperature $T_c$ at which the free energies of both (the superconducting and the normal) phases are equal, can be then identified with the temperature of the superconducting phase transition.

After a detailed analysis of the free energy (cf. figure 2 as an example), it turns out that the free energy of the superconducting phase corresponding to the lower branch of the energy gap (an the chemical potential) is greater than the free energy of the normal phase in the whole temperature range $T_0 < T \leq T^*$. Therefore in this temperature range this branch is not physically significant. On the other
hand, the free energy corresponding to the upper branch of the solutions is smaller than the free energy of the normal phase for $0 \leq T < T_c$. For $T_c < T \leq T^*$ the free energy of the normal phase is smaller and the system stops to be superconducting. The temperature $T_c$, at which the free energies of both phases are equal, is therefore identified with the temperature of the phase transition between the normal and the superconducting phase [7,8,12-14].

Figure 2. The difference between the free energy of the superconducting and the free energy of the normal phase for the SFL in the critical region (the case $\omega/\Delta(0) = 2$ has been chosen as an example). The three characteristic temperatures are marked. The vertical dotted line is plotted to indicate the temperature of the phase transition.

These observations can be summarized as follows [7,13]. Although in the supercritical temperature range $T_c < T \leq T^*$ there is a non-zero solution of the equation for the chemical potential and the gap equation (which is a unique feature of the superconducting state) the system stays normal, because the free energy criterion chooses the normal phase as the stable one. The existence of a non-zero solution of the energy gap (chemical potential) equation in spite of the fact that the system as a whole is in the normal phase, points to a possibility of Cooper pairs formation even above the phase transition temperature $T_c$. This fact can be related to the emergence of a pseudogap within the following scenario. At the temperature $T^*$ phase incoherent Cooper pairs can be formed and the pseudogap opens. As a result of cooling the system further down to $T_c$ – when the normal phase becomes (in terms of the free energy) disadvantageous for the system – the preformed Cooper pairs gain the phase coherence and the systems undergoes a phase transition to the superconducting state. The values of the three characteristic temperatures $T_0 < T_c < T^*$ involved in this scenario are quoted in table 1.

**Table 1.** The values of the three characteristic temperatures in the pseudogap scenario (see also Ref. [7]).

| $\omega/\Delta(0)$ | $T_0/\Delta(0)$ | $T_c/\Delta(0)$ | $T^*/\Delta(0)$ |
|-------------------|-----------------|-----------------|-----------------|
| 2                 | 0.2958          | 0.3038          | 0.3061          |
| $2\sqrt{5}$       | 0.2022          | 0.2124          | 0.2151          |
| 10                | 0.1259          | 0.1339          | 0.1359          |

The pseudogap-like behaviour is not the only unusual signature of the superconducting phase in the SFL system. As already mentioned, having known the free energy of both phases, we are able to find other thermodynamic quantities characterizing the phase transition (cf. table 2). In particular, calculation of the entropy reveals its pronounced discontinuity at the phase transition, what could be already inferred from the form of the free energy presented in figure 2. Hence, the superconducting phase transition observed in the SFL system is of the first order [7,8,12].
Table 2. Some thermodynamic characteristics at the phase transition temperature [7].

| $\omega$ | $T_c$ | $\Delta(T_c)$ | $\mu_s(T_c)$ | $T_c\Delta S(T_c)$ |
|---------|-------|---------------|--------------|---------------------|
| $\Delta(0)$ | $\Delta(0)$ | $\Delta(0)$ | $\Delta(0)$ | $N(0)\Delta^2(0)$ |
| 2       | 0.3038 | 0.5320        | 0.1691       | 0.1719              |
| $2\sqrt{5}$ | 0.2124 | 0.4704        | 0.1301       | 0.1380              |
| 10      | 0.1339 | 0.3324        | 0.0888       | 0.0689              |

4. Magnetic field induced effects
In the present section we will briefly discuss some properties of the SFL placed in an external magnetic field. We will limit our discussion to two characteristics, namely the critical magnetic field and the magnetic field penetration depth. These two quantities, which are important in practical applications, represent the two opposite limits: of strong and weak magnetic fields, respectively. For a more detailed review of the effects induced by the magnetic field, including the spin susceptibility and the critical current, the reader is referred to our papers [7,11].

Having known the free energy values of both phases for $0 \leq T \leq T_c$ in the absence of any external fields [7,8] we are able to find the critical magnetic field $H_c$ as [7,11,13]

$$H_c(T) = \frac{F_S(T) - F_S(T)}{8\pi}. \quad (3)$$

The temperature dependence of the critical magnetic field is presented in Figure 3.

![Figure 3](image)

**Figure 3.** Critical magnetic field for the s-wave paired SFL with $\omega/\Delta(0) = 2$ (solid), $2\sqrt{5}$ (dashed), 10 (dotted) [7,11,13].

Rewriting equation (3) as $F_S(T) - F_S(T) = (8\pi)^{-1} H_c^2(T)$ and differentiating both sides with respect to the temperature, one obtains the formula

$$S_S(T) - S_S(T) = \frac{1}{4\pi} H_c(T) \frac{dH_c(T)}{dT}. \quad (4)$$
Note that the rhs of equation (4) is negative for all \(0 \leq T < T_c\). Hence, the superconducting phase is the phase of the lower entropy. Moreover, the heat of the magnetic-field-driven phase transition to the normal phase is non-zero in the discussed temperature range. Hence the phase transition is of the first order, similar to the situation for \(T = T_c\) and \(H = 0\) discussed in the previous section.

The analysis of the penetration depth, which is a quantitative measure of the Meissner effect, is more complicated. In order to proceed with it, one introduces the gauge-invariant superflow \(\vec{v} = \nabla \varphi - e\vec{A}/m\), where \(\vec{A}\) is the vector potential, \(\varphi\) is the phase of Cooper pairs wave-function and \(m\) is either the bare or the effective mass. The superflow has a physical meaning of the Cooper pair velocity [15] and its inclusion into the Hamiltonian is performed by the transformation \(\vec{k} \mapsto \vec{k} + mv\), where \(k >> mv\). Note that the total momentum of the Cooper pair is now \(2mv\), unlike in the absence of the magnetic field when it is zero. Therefore the basis of the 9-dimensional Fock space should be chosen as

\[
\psi_{\sigma'\sigma}(k) = \begin{pmatrix} k + mv, \sigma \\ -k + mv, \sigma' \end{pmatrix}
\]

where \(\sigma, \sigma' = 0, \uparrow, \downarrow\). Moreover, the chemical potential \(\mu \mapsto \mu - mv^2/2\), i.e. it is constant up to terms \(O(v^3)\).

However, in order to find the complete expression for the thermodynamic potential one should also take into account the energy of the magnetic field itself. The variation of the thermodynamic potential due to the vector potential turns to be \(\delta \Omega = -j \cdot \delta \vec{A}\), where \(j\) is the current of normal particles in the SFL system given (up to linear terms in the superflow) by the formula [7,11,15]

\[
j = \frac{e\beta}{2m} \sum_k \langle k|\vec{v}\rangle 4 \frac{1}{4 + 3e^{\mu_k} + 2\cosh \beta E_k},
\]

where \(E_k = \sqrt{\epsilon_k^2 + 2\Delta_k^2}\) and \(\beta = (k_B T)^{-1}\). The superconducting (Cooper pairs) current, the superflow and the current of normal particles obey the relation \(j_s = e\dot{N}v - j\), which can be rewritten as \(j_s = e\dot{N}v(1 - N_s(T)/N)\). Here \(N_s\) is the temperature-dependent number of normal (unpaired) particles, related to the magnetic field penetration depth \(\lambda(T)\) by the formula \([\lambda(0)/\lambda(T)]^2 = 1 - N_s(T)/N\) [16].

Note that \(N_s(0) = N\), as at \(T = 0\) all particles are paired. For the \(s\)-wave paired SFL the temperature dependence of the magnetic field penetration depth is presented in figure 4 [7,11,14].

**Figure 4.** Magnetic field penetration depth for the \(s\)-wave paired SFL with \(\omega/\Delta(0) = 2\) (solid), \(2\sqrt{2}\) (dashed), 10 (dotted) [7,11,14].
5. Conclusions
The detailed study of the critical temperature region presented in the paper has revealed a number of features which point to the fact that the superconducting phase of the SFL is not a standard one. In the system a kind of pseudogap behavior can be observed with a possibility of pre-formation of phase-incoherent Cooper pairs above the temperature $T_c$ of the superconducting phase transition. Moreover, unlike in a standard BCS system, the phase transition has been found to be of the first order with a pronounced discontinuity in the entropy.

The brief discussion of the effects induced by a weak external magnetic field showed that in the SFL system at the temperature infinitesimally smaller than $T_c$, the fraction of normal particles is small (and so is the penetration depth). This is in contrast with the typical BCS behavior, where the fraction of normal particles is infinitesimally close to one for a system infinitesimally below $T_c$.

Acknowledgements
One of the authors (MK) is grateful to Professor Shiping Feng for his kind hospitality at the Department of Physics, Beijing Normal University. MK was supported by the China Scholarship Council (CSC No. 2007616032). A research scholarship from Wroclaw University of Technology is also gratefully acknowledged.

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