Multiple scattering corrections to the $\mathcal{T}$-matrix approximation: Unified theory of normal and superconducting states

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(Received 15 July 2008; revised manuscript received 30 September 2008; published 5 December 2008)

We present unified theory of both normal and superconducting states based on the fully self-consistent $\mathcal{T}$-matrix approximation. We argue that the failure of the customary $\mathcal{T}$-matrix approach below the critical temperature is caused by nonphysical repeated collisions. We eliminated the repeated collisions from the Galitskii-Feynman approximation. Obtained corrections are proportional to the inverse volume in the normal state and, thus, vanish in the thermodynamical limit. In the superconducting state these corrections remain finite and describe the Bardeen-Cooper-Schrieffer (BCS) gap. The $\mathcal{T}$-matrix approach goes beyond mean-field BCS theory. It is, thus, well suited for studies of the systems with large fluctuations such as the BCS–Bose-Einstein-condensate crossover or size effects in small metallic grains and the nuclear matter.

DOI: 10.1103/PhysRevB.78.214506 PACS number(s): 71.10.−w, 03.75.Ss, 05.30.Fk, 74.20.−z

I. INTRODUCTION

Trapped Fermi gases with binary interaction controlled by an external magnetic field offer a laboratory for studies of the superconducting state under extremely versatile conditions.[1–6] The crossover from the Bardeen-Cooper-Schrieffer (BCS) superconductivity to the Bose-Einstein condensate (BEC) is one of newly accessed regimes. Experiments on these systems can test recent theoretical nonperturbative approaches[7–13] or quantum Monte Carlo simulations.[14,15]

Another "superconducting" phenomenon which has attracted a lot of attention is the pseudogap in high-T_c materials (see Refs. 16–18 and references therein). As follows from solutions of the Hubbard model,[16,19–23] the pseudogap is caused by precursor superconducting fluctuations. This behavior is beyond mean-field theories of the BCS type. It should be noted that the Hubbard model is also used to study the BCS-BEC crossover.[9,24]

Important role of superconducting fluctuations has revived an interest in low-dimensional systems. A decade ago the tunneling spectroscopy of metallic nanoparticles[25,26] has confirmed size effects predicted by Anderson.[27] Recent theoretical studies[6,28] benefit from the Richardson approach[29] designed originally for the size correction to superfluidity in nuclei.

It is a challenge for the many-body theory to develop approximations covering the superconducting phase transitions in such a wide family of systems. Most nonperturbative approaches,[10,13–16] however, represent rather special methods with difficult intuitive interpretations. Moreover, these methods do not provide a simple link to nonequilibrium phenomena.[30,31]

In this paper we employ the many-body Green's functions which have a convenient diagrammatic representation and a well-established interpretation. We work with Matsubara's functions, but the reader skilled in the Kadanoff-Baym or Keldysh formalism[32–35] can readily convert all present formulas into equations for the nonequilibrium Green's functions.

Our approach is based on the two-particle $\mathcal{T}$ matrix in the ladder approximation proposed by Galitskii[36] within Feynman's perturbation scheme.[37] It is useful for systems with strong interaction of short range, be it nucleons, ^{3}He atoms in quantum liquid, or any atoms in a gas.

We modify the Galitskii-Feynman approximation by removing nonphysical repeated collisions as demanded by the multiple-scattering theory.[38,39] With this technically minor modification the $\mathcal{T}$-matrix approximation becomes applicable to the superconducting state. In the (conventional) normal metal, corrections are of the order of $1/\Omega$, where Ω is a system volume, but in the superconductor these corrections are of the order of unity.

A. $\mathcal{T}$ matrix in the theory of superconductivity

Let us first outline why the Galitskii-Feynman approximation has to be modified. This is best seen from the history of its implementations.

Applications of the $\mathcal{T}$ matrix to the superconductivity have been attempted shortly after the invention of BCS theory because the $\mathcal{T}$ matrix describes two-particle correlations including bound states.[40,41] This method offers a natural way to establish parameters of the interaction Hamiltonian from experimental data. Indeed, in the low-density limit, the $\mathcal{T}$ matrix yields the differential scattering cross section, which provides the most sensitive experimental data on the interaction, be it for nucleons[42,43] or atoms in the gas. It should be noticed that interaction via the Feshbach resonance[11] is also treated in terms of the scattering cross section.

The application of the $\mathcal{T}$ matrix to the superconductivity turned out to be problematic, however. Among various perturbation schemes for many-body systems, only the Galitskii-Feynman method correctly describes the instability of the normal state with respect to a formation of Cooper pairs.[41,44] This success is only partial, however. Already in 1960 Prange[45] and Wild[46] showed that the Galitskii-Feynman $\mathcal{T}$ matrix diverges at the critical temperature as expected, but it fails to describe the BCS gap at lower temperatures.

Prange[45] pointed out that the BCS theory is recovered if one replaces all the dressed Green's functions of the closed loop by their bare (noninteracting) values while the open line of self-energy remains dressed. Properties of such partly self-consistent theory were discussed in detail by Kadanoff and Martin[47] and tested on the attractive Hubbard model,[10] showing that it yields satisfactory results for the superconducting state. Of course, this theory is not suited for the normal state for which one should use the fully self-consistent Galitskii-Feynman approximation.

The superiority of the unjustified partly self-consistent theory over the fully self-consistent Galitskii-Feynman approximation is striking. How can one trust theory in which inclusion of additional diagrams destroys fundamental physical properties? Tolmachev[48] calls this problem the Prange paradox.

Tolmachev saw the origin of the paradox in a violated Ward identity.[48] He proposed to leave the customary relation between the $\mathcal{T}$ matrix and the self-energy in which one closes the loop on one of lines of the $\mathcal{T}$ matrix. Instead he constructs the self-energy from the Ward identity. His scheme is rather complicated and as far as we know it was never implemented.

Langer[49] identifies the problem of the $\mathcal{T}$-matrix approach to superconductivity in a violated antisymmetry of many-particle states. He proposed to avoid the linked cluster expansion and evaluate the statistical sum by a direct summation. His inspirative approach is too complicated to be implemented.

Apparently, the $\mathcal{T}$-matrix theories are different for the normal and the superconducting state. Above the critical temperature the Galitskii-Feynman approximation covers the normal state including the pseudogap.[50] Below the critical temperature, the superconducting gap appears only within a partly non-self-consistent theory. To be able to study the phase transition itself and the fluctuations in its vicinity, it is desirable to have a theory which covers the normal and the superconducting states on the same footing.

With this aim several groups adopted the idea[40,51,52] designed for ^{3}He to extend the BCS theory by embedding the anomalous Green's functions into the two-particle propagation of the $\mathcal{T}$ matrix.[11,12,19,53,54] This modification turned out to cover a wide family of effects. It applies to the normal and superconducting states and it describes the BEC on the level of the Popov approximation,[55] i.e., it describes the BCS-BEC crossover. In the condensed state this theory includes fluctuations which reduce the critical temperature and lead to the pseudogap in the single-particle spectrum.

Customary theory of superconductivity based on the anomalous functions does not cover fluctuations of condensate. Gyorffy *et al.*[56] introduced the anomalous functions in the spirit of the Hubbard alloy analogy to include fluctuations beyond the Gor'kov decoupling. Their numerical study shows profound effects for moderately strong-interaction strength. Koh[57] made an alternative step beyond Gor'kov decoupling assuming more general correlations contributing to a dressed interaction line. Apparently, the choice of anomalous functions is a problem within advanced approximations.

In this paper we attack the problem of the unified theory starting from the normal state. We argue that the Galitskii-Feynman approximation includes nonphysical processes in which a collision of two selected particles is repeated without interference of a third particle. Such repeated processes are impossible in reality, and in the perturbation expansion they cancel if the antisymmetry of the many-body state is properly retained. Since it is virtually impossible to include all diagrams necessary for such compensation, we propose to eliminate these nonphysical processes by a simple constraint which does not complicate an implementation of the $\mathcal{T}$-matrix approximation. We will show that if the nonphysical repeated processes are removed, the Galitskii-Feynman approximation works equally well in the normal and the superconducting states.

B. Plan of the paper

We first introduce the Galitskii-Feynman approximation in Sec. II A. Then we identify nonphysical processes responsible for the failure of the $\mathcal{T}$-matrix approach below the critical temperature in Sec. II B. In Sec. III we show how to eliminate them.

In the Appendix we discuss the single-channel approximation of the present theory. It is shown that below the critical temperature it yields the BCS gap including finite-size corrections smearing the phase transition. Above the critical temperature, the original Galitskii-Feynman approximation is recovered for the infinite volume.

II. DEFICIENCY OF THE $\mathcal{T}$-MATRIX APPROACH

Let us identify nonphysical processes hidden in the Galitskii-Feynman approximation. We treat a system of electrons with the Hamiltonian

$$\hat{H} = \sum_{\mathbf{k}} \epsilon(\mathbf{k})(a^\dagger_{\uparrow\mathbf{k}} a_{\uparrow\mathbf{k}} + a^\dagger_{\downarrow\mathbf{k}} a_{\downarrow\mathbf{k}}) + \frac{1}{\Omega}\sum_{\mathbf{kpq}} \mathcal{V}_{\mathbf{q}}(\mathbf{p},\mathbf{k}) a^\dagger_{\downarrow\mathbf{q}-\mathbf{k}} a^\dagger_{\uparrow\mathbf{k}} a_{\uparrow\mathbf{p}} a_{\downarrow\mathbf{q}-\mathbf{p}}. \quad (1)$$

We omit interactions between equal spins for simplicity. The kinetic energy has zero at the Fermi surface, $\epsilon(\mathbf{k}) = k^2/2m - E_F$. Variables $\mathbf{p}$ and $\mathbf{k}$ are the relative momenta before and after interaction, respectively. $\mathbf{q}$ is the total momentum of the interacting pair of particles. The creation $a^\dagger_{\uparrow\mathbf{k}}$ and annihilation $a_{\uparrow\mathbf{k}}$ operators are normalized to the sample (or quantization) volume Ω, e.g., $\psi^\dagger(\mathbf{r}) = (1/\sqrt{\Omega})\Sigma_{\mathbf{k}} a^\dagger_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}}$.

The dressed single-particle Green's function $G_\uparrow$ is given by the Dyson equation

$$G_\uparrow(\omega,\mathbf{k}) = G^0_\uparrow(\omega,\mathbf{k}) + G^0_\uparrow(\omega,\mathbf{k})\Sigma_\uparrow(\omega,\mathbf{k})G_\uparrow(\omega,\mathbf{k}) \quad (2)$$

with the bare Green's function

$$G^0_\uparrow(\omega,\mathbf{k}) = \frac{1}{i\omega - \epsilon(\mathbf{k})}. \quad (3)$$

Here Σ is the self-energy, i.e., an energy-dependent potential which simulates averaged effects of all electrons on the motion of a selected electron of momentum $\mathbf{k}$, spin $\uparrow$, and the Matsubara frequency ω.

A. Galitskii-Feynman approximation

The Galitskii-Feynman self-energy is constructed from the two-particle $\mathcal{T}$ matrix

$$\Sigma_{\uparrow}^{\mathrm{GF}}(\omega,\mathbf{k}) = \frac{k_B T}{\Omega}\sum_{z\mathbf{q}} \mathcal{T}_{\mathbf{q}}^{\mathrm{GF}}(z,\mathbf{k},\mathbf{k}) G_{\downarrow}(z-\omega,\mathbf{q}-\mathbf{k}). \quad (4)$$

In the ladder approximation the $\mathcal{T}$ matrix is

$$\mathcal{T}_{\mathbf{q}}^{\mathrm{GF}}(z,\mathbf{p},\mathbf{k}) = \mathcal{V}_{\mathbf{q}}(\mathbf{p},\mathbf{k}) - \frac{1}{\Omega}\sum_{\mathbf{k}'} \mathcal{V}_{\mathbf{q}}(\mathbf{p},\mathbf{k}')\mathcal{G}_{\mathbf{q}}^{\mathrm{GF}}(z,\mathbf{k}')\mathcal{T}_{\mathbf{q}}^{\mathrm{GF}}(z,\mathbf{k}',\mathbf{k}), \quad (5)$$

where

$$\mathcal{G}_{\mathbf{q}}^{\mathrm{GF}}(z,\mathbf{p}) = k_B T\sum_{\omega} G_{\uparrow}(\omega,\mathbf{p}) G_{\downarrow}(z-\omega,\mathbf{q}-\mathbf{p}) \quad (6)$$

describes the propagation of the two particles or holes during the collision. The convention of signs follows Abrikosov, Gor'kov, and Dzyaloshinski.[58]

B. Repeated collisions in the Galitskii-Feynman approximation

Let us show that the Galitskii-Feynman approximation includes nonphysical processes. First, there are repeated scattering-out processes which appear due to products of the self-energy in the Dyson Eq. (2). Indeed, if we expand the dressed function in powers of the self-energy, $G_{\uparrow}=G_{\uparrow}^0 + G_{\uparrow}^0\Sigma_{\uparrow}G_{\uparrow}^0 + G_{\uparrow}^0\Sigma_{\uparrow}G_{\uparrow}^0\Sigma_{\uparrow}G_{\uparrow}^0 + \cdots$, there is no restriction on repeated processes in products such as

$$G_{\uparrow}^0\Sigma_{\uparrow}G_{\uparrow}^0\Sigma_{\uparrow}G_{\uparrow}^0 = \frac{k_B^2 T^2}{\Omega^2} G_{\uparrow}^0 \sum_{z\mathbf{q}} (\mathcal{T}_{\mathbf{q}} G_{\downarrow}) G_{\uparrow}^0 \sum_{z'\mathbf{q}'} (\mathcal{T}_{\mathbf{q}'} G_{\downarrow}) G_{\uparrow}^0. \quad (7)$$

To avoid nonphysical repeated collisions, all products with $\mathbf{q}'=\mathbf{q}$ ought to be excluded.

Second, repeated scattering-in processes are hidden in the self-consistent construction of the self-energy. The self-energy is a functional of the dressed Green's functions, $\Sigma_{\uparrow}^{\mathrm{GF}}[G_{\uparrow},G_{\downarrow}]$ [see Eqs. (4)–(6)]. In this way the collision process described by the self-energy $\Sigma_{\uparrow}^{\mathrm{GF}}[G_{\uparrow},G_{\downarrow}]$ also contributes to its internal Green's function $G_{\uparrow}$; therefore, this process supplies particles into its own initial state. For instance, the self-energy [Eq. (4)] includes the double sum

$$\Sigma_{\uparrow}^{\mathrm{GF}}[G_{\uparrow},G_{\downarrow}] = \frac{k_B T}{\Omega}\sum_{z\mathbf{q}} \left(\mathcal{T}_{\mathbf{q}} \left[G_{\uparrow}^0 + G_{\uparrow}^0 \frac{k_B T}{\Omega} \sum_{z'\mathbf{q}'} (\mathcal{T}_{\mathbf{q}'} G_{\downarrow}) G_{\uparrow}^0 + , \ldots , G_{\downarrow} \right] G_{\downarrow} \right) \quad (8)$$

from which the terms with $\mathbf{q}'=q$ should be excluded.

We show below that in the normal metal, the repeated collisions yield negligible contribution, since the weight of a single channel in the sum over $\mathbf{q}$ is inversely proportional to the volume and vanishes in thermodynamical limit. In the superconductor, however, the repeated collisions in the pairing channel are enhanced and block the formation of the gap. Our goal is to remove these nonphysical processes from the perturbation expansion.

III. ELIMINATION OF THE REPEATED COLLISIONS

The simplest way to remove nonphysical processes is to sacrifice the whole classes of diagrams which include them. This is the physical reason for the success of the partly non-self-consistent approximation introduced by Prange[45] and recently called the Kadanoff-Martin approximation. Unfortunately, the classes of neglected diagrams are so large that this approximation does not describe the normal state.

In this section we introduce a constraint which removes the nonphysical processes selectively. We obtain a theory which equally well describes the normal and the superconducting states.

The perturbation expansion for multiple scattering without repeated collisions has been formulated within the nuclear physics (see Ref. 39 and references therein). These expansions (e.g., Fadeev equations) are suited for a small number of particles; therefore, they cannot be easily modified to condensed-matter problems.

The repeated collisions have also troubled the theory of alloys.[59,60] The straightforward summation of ladder diagrams for interaction of an electron with a single impurity leads to the so-called self-consistent averaged $\mathcal{T}$-matrix approximation, which has basically the same shortcomings as the Galitskii-Feynman $\mathcal{T}$-matrix approximation. In particular, an electron can be scattered by the same impurity twice without interference of any additional impurity. Similarly as we have seen above, such repeated scattering-out processes result from the powers of the self-energy in the Dyson equation and the repeated scattering-in processes results from the self-consistency of the $\mathcal{T}$ matrix.

Soven[59] showed that the repeated collisions are eliminated if the self-energy is defined via an effective medium. This should be distinguished from the usual approach, where the self-energy is expressed as a sum of selected diagrams. The sum of ladder diagrams for impurity embedded in the effective medium yields an approximation which is free of repeated collisions and provides appreciably better description of alloys than the averaged $\mathcal{T}$ matrix.[60]

The Soven idea of how to remove the repeated collisions can be adopted to the Galitskii-Feynman approximation as follows:

(i) Split the interaction and the self-energy into channels.

(ii) Describe all channels but one by the self-energy. For the selected channel use the collision theory to evaluate the $\mathcal{T}$ matrix.

(iii) Evaluate the Green's function from the $\mathcal{T}$ matrix. Identify the self-energy from the resulting Green's function.

Next we apply steps (i)–(iii).

(i) The interaction potential is naturally split into channels belonging to the total momentum $\mathbf{q}$. In analogy with Eq. (4) we can also expect that the self-energy is a sum of individual single-channel contributions

$$\Sigma_\uparrow(\omega,\mathbf{k}) = \sum_{\mathbf{q}} \Sigma_{\mathbf{q}\uparrow}(\omega,\mathbf{k}). \tag{9}$$

(ii) We define a subsidiary reduced Green's function in which the $\mathbf{q}$ channel is not included

$$G_{\mathbf{q}\uparrow} = G_\uparrow - G_{\mathbf{q}\uparrow}\Sigma_{\mathbf{q}\uparrow}G_\uparrow. \tag{10}$$

In terms of the bare Green's function the reduced Green's function reads $G_{\mathbf{q}\uparrow}=G^0_\uparrow+G_{\mathbf{q}\uparrow}(\Sigma_\uparrow-\Sigma_{\mathbf{q}\uparrow})G^0_\uparrow$.

From the $\mathbf{q}$-reduced Green's function we construct the $\mathbf{q}$-reduced two-particle Green's function

$$\mathcal{G}_{\mathbf{q}\uparrow}(z,\mathbf{p}) = k_B T\sum_\omega G_{\mathbf{q}\uparrow}(\omega,\mathbf{p})G_\downarrow(z-\omega,\mathbf{q}-\mathbf{p}). \tag{11}$$

Note that the Green's function for the spin $\downarrow$ is not reduced, because we have excluded only the spin $\uparrow$ part of the self-energy. The reduced spin component is specified in the subscript of the two-particle function.

The two-particle Green's function describes the intermediate propagation of two interacting particles in the ladder approximation of the $\mathcal{T}$ matrix

$$\mathcal{T}_{\mathbf{q}\uparrow}(z,\mathbf{p},\mathbf{k}) = \mathcal{V}_{\mathbf{q}}(\mathbf{p},\mathbf{k}) - \frac{1}{\Omega}\sum_{\mathbf{k}'} \mathcal{V}_{\mathbf{q}}(\mathbf{p},\mathbf{k}')\mathcal{G}_{\mathbf{q}\uparrow}(z,\mathbf{k}')\mathcal{T}_{\mathbf{q}\uparrow}(z,\mathbf{k}',\mathbf{k}). \tag{12}$$

Using the $\mathbf{q}$-reduced Green's function for the internal two-particle propagation, we have eliminated the repeated scattering-in processes.

(iii) The $\mathcal{T}$ matrix covers all orders of the binary interaction. The dressed Green's function, thus, reads

$$G_\uparrow(\omega,\mathbf{k}) = G_{\mathbf{q}\uparrow}(\omega,\mathbf{k}) + G_{\mathbf{q}\uparrow}(\omega,\mathbf{k})S_{\mathbf{q}\uparrow}(\omega,\mathbf{k})G_{\mathbf{q}\uparrow}(\omega,\mathbf{k}), \tag{13}$$

where

$$S_{\mathbf{q}\uparrow}(\omega,\mathbf{k}) = \frac{k_B T}{\Omega}\sum_z \mathcal{T}_{\mathbf{q}\uparrow}(z,\mathbf{k},\mathbf{k})G_\downarrow(z-\omega,\mathbf{q}-\mathbf{k}) \tag{14}$$

is the reducible self-energy for the channel $\mathbf{q}$. The reducible self-energy S has to be distinguished from the irreducible self-energy Σ. This construction is free of successive scattering-out collisions.

The irreducible self-energy Σ results when we express the dressed Green's function G from Eq. (10) and compare it with relation (13), $S_{\mathbf{q}\uparrow}=\Sigma_{\mathbf{q}\uparrow}(1-G_{\mathbf{q}\uparrow}\Sigma_{\mathbf{q}\uparrow})^{-1}$. This is solved by

$$\Sigma_{\mathbf{q}\uparrow}(\omega,\mathbf{k}) = \frac{S_{\mathbf{q}\uparrow}(\omega,\mathbf{k})}{1+G_{\mathbf{q}\uparrow}(\omega,\mathbf{k})S_{\mathbf{q}\uparrow}(\omega,\mathbf{k})}. \tag{15}$$

Equations (9)–(15) determine the self-energy $\Sigma[G]$ as a function of the dressed Green's function. The Dyson Eq. (2) gives $G[\Sigma]$ and closes the set of equations.

Numerical demands to solve the present set of equations are comparable to the solution of the Galitskii-Feynman $\mathcal{T}$-matrix approximation. Such a numerical treatment goes beyond the scope of this paper, however. In the Appendix we discuss properties of the present approximation under simplified conditions, which allow us to derive analytic results.

IV. SUMMARY

We have shown that the single-particle Green's function constructed from the two-particle $\mathcal{T}$ matrix includes nonphysical repeated collisions of interacting pairs. These nonphysical processes are negligible in the normal state but make the $\mathcal{T}$-matrix approach inapplicable to the superconducting state. We have eliminated the repeated collisions using ideas of the multiple-scattering theory. The present approximation reproduces the Galitskii-Feynman approximation in the normal state.

In the single-channel approximation the present theory reproduces the BCS results and provides a correction beyond it. This correction is inversely proportional to the sample volume and, thus, vanishes in the thermodynamic limit. At the finite volume this correction makes the transition from the normal to the superconducting state smooth, i.e., without nonanalytic jump at the transition temperature.

It is noteworthy that the present approach is not of the mean-field type and does not introduce anomalous functions. Since the theory is based on quantities corresponding to the mean value of the square of the gap, it includes fluctuations beyond the mean-field picture.

The present theory is based on the self-consistent expansion within the Green's functions. It is, thus, a suitable approximation for studies of the transport using the machinery of the nonequilibrium Green's functions.

ACKNOWLEDGMENTS

The author is grateful to Asle Sudbø and Pei-Jen Lin for fruitful discussions, and to František Šanda for a critical reading of the manuscript. This work was supported by Research No. MSM 0021620834, by Grants No. GAČR 202/07/0597 and No. GAAV 100100712, by PPP project of DAAD, and by European ESF program NES.

APPENDIX: BCS GAP WITH VOLUME CORRECTIONS

In this appendix we demonstrate the present theory on a simple model using additional approximations.

1. Single-channel approximation

Our discussion is restricted to homogeneous systems; therefore, there is no diamagnetic current and the Cooper pairs condense into the $\mathbf{q}=0$ state. We, thus, expect $\Sigma_{\mathbf{q}=0} \gg \Sigma_{\mathbf{q}\neq 0}$ and write the self-energy as

$$\Sigma = \Sigma_0 + \sum_{\mathbf{q}\neq 0} \Sigma_{\mathbf{q}} = \Sigma_0 + \Sigma'. \tag{A1}$$

We focus on the $\mathbf{q}=0$ and spin $\uparrow$ channel. By definition, the 0-reduced Green's function is

$$G_{0\uparrow}(\omega,\mathbf{k}) = \frac{1}{i\omega - \epsilon(\mathbf{k}) - \Sigma'_{\uparrow}(\omega,\mathbf{k})}, \tag{A2}$$

and the Dyson equation yields the dressed function as

$$G_{\uparrow}(\omega,\mathbf{k}) = \frac{1}{i\omega - \epsilon(\mathbf{k}) - \Sigma'_{\uparrow}(\omega,\mathbf{k}) - \Sigma_{0\uparrow}(\omega,\mathbf{k})}. \tag{A3}$$

We remind that the subscript with bold face 0 denotes the $\mathbf{q}=0$ channel. It should be distinguished from the superscript 0 which above denotes the bare function, $G^0 \neq G_0$. Within this appendix the bare function is not used.

Due to the singular character of the Bose statistics, the zero-frequency element of the $\mathcal{T}$ matrix is much larger than others, $\mathcal{T}_0(z=0,\mathbf{k},\mathbf{k}) \gg \mathcal{T}_0(z\neq 0,\mathbf{k},\mathbf{k})$. Neglecting the nonzero frequencies we approximate the reducible self-energy as

$$S_{0\uparrow}(\omega,\mathbf{k}) \approx \frac{k_B T}{\Omega} \mathcal{T}_0(0,\mathbf{k},\mathbf{k}) G_{\downarrow}(-\omega,-k). \tag{A4}$$

The reducible self-energy [Eq. (A4)] can be readily substituted into the dressed Green's function [Eq. (13)]. Since the reducible self-energy $S_{0\downarrow}$ is obtained by the interchange $\uparrow \leftrightarrow \downarrow$ in the above expression, the set of equations is closed. The resulting dressed Green's function reads

$$G_{\uparrow}(\omega,\mathbf{k}) = \frac{1}{i\omega - \epsilon(\mathbf{k}) - \Sigma'_{\uparrow}(\omega,\mathbf{k}) - \dfrac{\dfrac{k_B T}{\Omega}\mathcal{T}_{0\uparrow}(0,\mathbf{k},\mathbf{k})}{-i\omega - \epsilon(-\mathbf{k}) - \Sigma'_{\downarrow}(-\omega,-\mathbf{k})}}. \tag{A5}$$

2. Energy gap

The single-particle excitation energy is given by the pole of G. In order to proceed on a simple analytic level, we approximate the regular part of the self-energy in the spirit of the quasiparticle picture by the correction to the band structure,

$$\epsilon(\mathbf{k}) + \Sigma'_{\uparrow}(\omega,\mathbf{k}) \approx \xi(\mathbf{k}). \tag{A6}$$

In the quasiparticle approximation [Eq. (A6)] the Green's function [Eq. (A5)] results as

$$G_{\uparrow}(\omega,\mathbf{k}) = \frac{-i\omega - \xi(-\mathbf{k})}{\omega^2 + \xi^2(\mathbf{k}) - \dfrac{k_B T}{\Omega}\mathcal{T}_{0\uparrow}(0,\mathbf{k},\mathbf{k})}. \tag{A7}$$

The single-particle excitation energy (given by roots of the denominator with respect to $i\omega$) has two branches

$$\varepsilon_{\uparrow}(\mathbf{k}) = \pm \sqrt{\xi^2(\mathbf{k}) - \frac{k_B T}{\Omega}\mathcal{T}_{0\uparrow}(0,\mathbf{k},\mathbf{k})} \tag{A8}$$

with the gap

$$\Delta_{\uparrow}(\mathbf{k}) = \sqrt{-\frac{k_B T}{\Omega}\mathcal{T}_{0\uparrow}(0,\mathbf{k},\mathbf{k})}. \tag{A9}$$

Relation (A9) between the gap and the singular element of the $\mathcal{T}$ matrix holds for a general interaction potential $\mathcal{V}$, provided that $\mathcal{V}$ leads to pairing.

3. Gap equation

To find at which temperature the Cooper pairs nucleate and how strong their condensate is below this temperature requires specifying the interaction potential. An explicit condition for the gap, the so-called gap equation, can be derived using the separable BCS potential

$$\mathcal{V}_0(\mathbf{p},\mathbf{k}) = -V\theta(\omega_{\mathrm{cut}} - |\xi(\mathbf{p})|)\,\theta(\omega_{\mathrm{cut}} - |\xi(\mathbf{k})|). \tag{A10}$$

The negative sign in the potential corresponds to a convention of the BCS theory.[61] The $\mathcal{T}$ matrix is then also separable

$$\mathcal{T}_{0\uparrow}(0,\mathbf{p},\mathbf{k}) = \mathcal{T}_0(0)\,\theta(\omega_{\mathrm{cut}} - |\xi(\mathbf{p})|)\,\theta(\omega_{\mathrm{cut}} - |\xi(\mathbf{k})|). \tag{A11}$$

Equation (12) now achieves a simple algebraic form

$$\mathcal{T}_0(0) = -V + V\frac{1}{\Omega}\sum_{\mathbf{k}}^{|\xi(\mathbf{k})|<\omega_{\mathrm{cut}}} \mathcal{G}_0(0,\mathbf{k})\mathcal{T}_0(0), \tag{A12}$$

which can be rewritten as

$$\frac{1}{V} - \frac{1}{\Omega}\sum_{\mathbf{k}}^{|\xi(\mathbf{k})|<\omega_{\mathrm{cut}}} \mathcal{G}_0(0,\mathbf{k}) = -\frac{1}{\mathcal{T}_0(0)}. \tag{A13}$$

Condition (A13) corresponds to the BCS gap equation. To see this we evaluate the integral over the two-particle Green's function

$$\mathcal{J}=\frac{1}{\Omega}\sum_{\mathbf{k}}^{|\xi(\mathbf{k})|<\omega_{\mathrm{cut}}}\mathcal{G}_0(0,\mathbf{k})=\frac{k_BT}{\Omega}\sum_{\omega\mathbf{k}}^{|\xi(\mathbf{k})|<\omega_{\mathrm{cut}}}G_{0\uparrow}(\omega,\mathbf{k})G_{\downarrow}(-\omega,-\mathbf{k})$$

$$=\frac{k_BT}{\Omega}\sum_{\omega\mathbf{k}}^{|\xi(\mathbf{k})|<\omega_{\mathrm{cut}}}\frac{1}{\omega^2+\xi^2(\mathbf{k})-\frac{k_BT}{\Omega}\mathcal{T}_0(0)}. \tag{A14}$$

In the first step we have substituted the two-particle function $\mathcal{G}_0$ from its definition [Eq. (11)]. In the second step the single-particle Green's function [Eq. (A7)] and reduced Green's function [Eq. (A2)] in the quasiparticle approximation [Eq. (A6)] have been used.

The sum over momenta can be expressed in terms of the density of states

$$N_E=\frac{1}{\Omega}\sum_{\mathbf{k}}\delta[E-\xi(\mathbf{k})] \tag{A15}$$

as

$$\mathcal{J}=k_BT\int_{-\omega_{\mathrm{cut}}}^{\omega_{\mathrm{cut}}}dE\frac{N_E}{\omega^2+E^2-\frac{k_BT}{\Omega}\mathcal{T}_0(0)}. \tag{A16}$$

Finally, we express the $\mathcal{T}$ matrix via the gap using relation (A9)

$$\Delta^2=-\frac{k_BT}{\Omega}\mathcal{T}_0(0) \tag{A17}$$

so that condition (A13) reads

$$\frac{1}{V}-k_BT\int_{-\omega_{\mathrm{cut}}}^{\omega_{\mathrm{cut}}}dE\sum_z\frac{N_E}{z^2+E^2+\Delta^2}=\frac{k_BT}{\Omega\Delta^2}. \tag{A18}$$

The sum over Matsubara frequencies $z=(2n+1)\pi k_BT$ can be easily evaluated and leads to the distribution, $k_BT\Sigma_z\frac{1}{z^2+\varepsilon^2}=\frac{1}{2\varepsilon}\tanh\frac{\varepsilon}{2k_BT}$. Condition (A18) turns into the gap equation

$$\frac{1}{V}-\int_{-\omega_{\mathrm{cut}}}^{\omega_{\mathrm{cut}}}\frac{N_EdE}{2\sqrt{E^2+\Delta^2}}\tanh\frac{\sqrt{E^2+\Delta^2}}{2k_BT}=\frac{k_BT}{\Omega\Delta^2}. \tag{A19}$$

In the thermodynamical limit $\Omega\to\infty$ the right-hand side goes to zero so that Eq. (A19) reduces to the familiar gap equation of Bardeen, Cooper, and Schrieffer. It should be noted that the correction is proportional to the temperature, i.e., the zero-temperature gap studied in Refs. 62–64 is not modified in the present approximation.

4. Volume corrections to the BCS gap equation

In nanometer-scale metallic grains the density of states N_E is a sum of delta functions at discrete energy levels. The mean energy distance η of the levels on the scale of the zero-temperature BCS gap Δ_0 controls the size effect on the superconductivity.[27] For $\eta/\Delta_0\to 0$ one finds the BCS gap, while for $\eta/\Delta_0>1$ the superconductivity disappears. This effect has been experimentally confirmed and basic features are qualitatively understood from the Richardson model (see Ref. 26 and references therein). Quantitative studies of the volume and shape dependence of the gap are based on the BCS theory.[62–64]

Equation (A19) parallels the BCS gap equation; therefore, it covers effects of the discrete energy spectrum,[63,64] changes of the effective interaction due to finite extent of the single-electron wave functions,[62] and eventual surface enhancement of the superconductivity.[62] Besides it includes an additional volume correction given by the term on the right-hand side. To make clear the role of this new term, we neglect all the above-mentioned effects and assume a constant density of states near the Fermi level, $N_E\approx N_0$.

The volume correction is important in the vicinity of the critical temperature, where the gap is small and the correction term on the right-hand side of the gap [Eq. (A19)] becomes sizable. Let us focus on the vicinity of the critical temperature.

Close to the critical temperature the integral on the left-hand side of Eq. (A19) can be expanded in powers of the gap

$$\frac{1}{V}-N_0\int_0^{\omega_{\mathrm{cut}}}\frac{dE}{\sqrt{E^2+\Delta^2}}\tanh\frac{\sqrt{E^2+\Delta^2}}{2k_BT}\approx N_0\left(\frac{T}{T_c}-1+\frac{\Delta^2}{\Delta_0^2}\right). \tag{A20}$$

The same expansion is used in the microscopic derivation of the Ginzburg-Landau theory from the BCS theory.[65]

Within approximation (A20) the gap [Eq. (A19)] is a quadratic equation for Δ^2 with the positive root

$$\Delta^2=\frac{\Delta_0^2}{2}\left(\left(1-\frac{T}{T_c}\right)+\sqrt{\left(1-\frac{T}{T_c}\right)^2+\frac{4k_BT_c}{\Omega N_0\Delta_0^2}}\right). \tag{A21}$$

In formula (A21) one can see that the transition from the normal to the superconducting state is smeared on the temperature scale proportional to the inverse volume.

Sufficiently below the critical temperature, formula (A21) yields the finite gap,

$$\Delta^2\approx\Delta_0^2\left(1-\frac{T}{T_c}\right) \tag{A22}$$

for $T_c-T\gg\sqrt{\frac{4k_BT_c^3}{\Omega N_0\Delta_0^2}}$. The finite-volume correction is negligible compared to the gap in this regime.

The small parameter $4k_BT_c/(\Omega N_0\Delta_0^2)$ determines the width of the phase transition. Since the density of states relates to the mean distance of energy levels, $\Omega N_0=1/\eta$, and the critical temperature relates to the gap, $k_BT_c=(4/7)\Delta_0$, we

can express this width of transition as $4k_BT_c/(\Omega N_0\Delta_0^2) = (16/7)\eta/\Delta_0$. This form shows that the term on the right-hand side of the gap [Eq. (A19)] becomes important for the same sample sizes as the discrete structure of energy levels.

5. Recovering the Galitskii-Feynman approximation in the normal state

Finally, we take a look on the meaning of the gap [Eq. (A19)] above the critical temperature. We restrict our attention to the vicinity of the critical temperature where the approximative solution [Eq. (A21)] holds.

Sufficiently above the critical temperature the single-channel $\mathcal{T}$ matrix resulting from Eq. (A21) is inversely proportional to the volume,

$$\mathcal{T}_{0\uparrow} = -\frac{\Delta^2}{k_BT} \approx \frac{k_BT_c}{\Omega N_0\left(1-\frac{T}{T_c}\right)} \tag{A23}$$

for $T-T_c \gg \sqrt{\frac{4k_BT_c^3}{\Omega N_0\Delta_0^2}}$. Its contribution to the self-energy is thus not singular and there is no gap. From Eq. (15) it follows that in the thermodynamic limit, $\Omega\to\infty$, the reducible and irreducible single-channel self-energies become identical, $\Sigma_{\mathbf{q}\uparrow}\to S_{\mathbf{q}\uparrow}$, for all values of $\mathbf{q}$. At the same time, the single-channel self-energy makes only negligible correction to the Green's function, $G_{\mathbf{q}\uparrow}\to G_\uparrow$, therefore $\mathcal{G}_{\mathbf{q}\uparrow}\to\mathcal{G}_{\mathbf{q}}^{\mathrm{GF}}$. In the normal state the present approximation is, thus, identical to the Galitskii-Feynman approximation.

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