Self-consistent T-matrix theory of superconductivity

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Using principles of the Fadeev-Lovelace-Watson multiple scattering expansion, a T-matrix approximation is derived which coincides with the Galitskii-Feynman T matrix in the normal state and yields the gap in the superconducting state. Unlike other T-matrix approaches, the theory satisfies not only the self-consistent Thouless criterion but also the Baym-Kadanoff conditions for a conserving theory in equilibrium. In single-mode approximation it simplifies to the Eliashberg theory.

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I. INTRODUCTION

The known family of superconducting materials contains such diverse systems as conventional metals and metallic alloys,[1] high-T_c ceramics,[2] fullerenes,[3] organic superconductors,[4] doped diamond,[5] heavy fermion metals,[6] He-III (Ref. 7), symmetric nuclear matter,[8–10] and very asymmetric nuclear matter in neutron stars,[11] Fermi gases,[12] as well as hypothetical condensates like the color superconductivity of quarks.[13] It is rather surprising how many features of these systems have been successfully explained within the mean-field BCS theory and its Green's-function extension due to Eliashberg. On the other hand, there is a growing list of experimental facts which require the employment of more elaborate theories.

Recent theoretical approaches to superconductivity range from the trial wave functions of Gutzwiller type,[14] to improved Eliashberg theories,[15] renormalization group approaches within path integrals,[16] exact diagonalizations and quantum Monte Carlo studies[17] on simple models having small size or infinite dimensions,[18] and the many-body T-matrix approximations[19–25] and hybrid theories combining the anomalous functions of Eliashberg type either with the many-body T matrix[26,27] or with the fluctuation-exchange approximation.[28–30]

The formulation we present in the following is not of any of the types mentioned above. We recall Watson's multiple scattering theory;[31,32] his ideas were used by Fadeev[33–35] and Lovelace[36] in their description of few-body systems. In these small systems it is crucial that each subsequent collision of a particle be with a different partner; this is because the two-particle T matrix covers the binary interaction to all orders.[37]

This obvious physical principle is generally difficult to implement in diagrammatic expansion methods, since generically the Feynman rules do not impose any conditions on subsequent events; a summation obtains over all possible partners. Similarly, one does not find any corresponding restriction of partners in the renormalization group approaches.

A nonphysical repetition of collisions with the same partner does not introduce problems for normal metals, because the weight of repeated collisions in unrestricted summations scales with the reciprocal number of particles. This is in contrast to the case of superconductors, where the condensate breaks this scaling behavior for pairing interactions and the nonphysical repetition becomes a serious problem. In Ref. 38 one of the present authors was able to eliminate the repeated collisions from the Galtskii-Feynman approximation[39] using Soven's concept of the effective medium.[40] The Soven-type corrections are negligible in the normal metal but become significant when the condensate develops. The approach proposed in Ref. 38 applies only to systems with a nonretarded interaction. For many of the systems listed above, however, the retarded nature of interaction is an essential ingredient of a theoretical model if the goal is to achieve quantitative agreement with experiment. The main focus of the present paper is to derive a T-matrix approximation engineered for many-fermion systems with pairing mediated by bosons; that is, with a retarded interaction of finite range.

It is desirable that the theory be conserving in the Baym-Kadanoff sense.[41] Methods which depend upon the introduction of anomalous functions face great difficulty in this respect, as the Baym-Kadanoff symmetry conditions are very restrictive. It may be pointed out that anomalous functions themselves generically violate particle-number conservation on the microscopic scale. It will be seen shortly that in our formulation anomalous functions are not introduced but instead appear as a consequence of other less disruptive ingredients. Anomalous functions may be considered an approximation of the two-particle Green's function when the T matrix develops a singular separable term below the critical temperature. This separable form constitutes a significant simplification, confirming the vital role of anomalous functions in the theory of superconductivity.

Theories starting with anomalous functions treat processes forming the condensate nonperturbatively,[42,43] while other processes are covered by low-order approximations. In a construction free of anomalous functions, all binary interactions may be described to the same approximation, enabling the expression of exact conservation laws.

It is known that the superconducting gap cannot be obtained in the framework of what is referred to as a *self-consistent* Feynman diagrammatic expansion. It is also true that self-consistency is a requirement of conserving theories. The problem this poses is parallel to the conserving-gapless dichotomy in the theory of Bose condensates.[26] In the approach of the present paper, this problem is absent; the Baym-Kadanoff conditions for conservation are satisfied, but not at the expense of the superconducting gap.

In fact, Lorentz already in 1869 had some ideas which guide us on the correct path; the problem with the theory may be identified as the presence of nonphysical self-interactions, and the idea is to excise these in a consistent way. Looking at the issue from a different viewpoint, the issue can be understood in terms of unphysical repeated collisions; elimination of these is the major achievement of the Fadeev-Lavelace-Watson multiple scattering approach, which is also capable of producing a superconducting gap.[38] The first approach is more intuitive; the second approach supports more rigorous justification. In this paper we present both before showing that they are, in fact, equivalent. We refer to the resulting theory as *restricted self-consistent*, or RSC.

The paper is organized as follows. In Sec. II we set the stage by reviewing the T-matrix approaches, comparing the Galitskii-Feynman[39,44] (GF) and the Kadanoff-Martin[19] (KM) approximations. We discuss the issue of self-interactions in the GF approach and the problem of the Thouless criterion in the KM approach, thus illustrating the need for a novel treatment suffering the problems of neither. In Sec. III we introduce the idea of restricted self-consistency, by which we intuitively construct a system of equations describing our new approach while avoiding the complexity of the multiple scattering theory; the result is the RSC theory. In Sec. IV we begin to analyze this theory, showing the appearance of the gap and also the normal-state coincidence with the GF theory. The separable approximation of the singular part of the T matrix is shown to lead to the Eliashberg theory. In Sec. V we prove that the two-particle Green's function in the RSC theory satisfies the conditions of Baym and Kadanoff for theories to be conserving on the microscopic level. Next, in Sec. VI we turn our attention to a derivation of a T-matrix approximation from the multiple scattering theory. After this is established, it is shown that this actually amounts to a more rigorous derivation of the same RSC theory constructed in Sec. III.

II. DIAGRAMMATIC T-MATRIX APPROACHES AND PROBLEMS

In this section we begin by reviewing some ideas about self-consistency and self-interaction and discuss the need for restricted self-consistency. We proceed to consider the concept of self-interactions mediated by the condensate, the issue of repeated collisions, and the problem of mutual exclusivity of self-consistency and appearance of the gap. The T-matrix theory can either be constructed via a so-called partly self-consistent or fully self-consistent diagrammatic expansion. We conclude this section by discussing both of these and pointing out why neither approach in fact produces a satisfactory theory, a problem which we resolve in Sec. III.

A. Lorentz self-consistency

A standard starting point is the search for functionals of the bare or dressed Green's functions, $\Sigma[G_0]$ or $\Sigma[G]$. Actually, neither G_0 nor G is suited to describe a single collision isolated from the series of collisions a given particle undergoes in the many-body system. This problem of self-consistency was first discussed by Lorentz in 1869. As his analysis is based on the well-understood electric field and allows for a transparent explanation, we review it here before applying such ideas to superconductivity. Lorentz theory is covered in detail by Chapter 13 of Kittel's textbook.[45]

Lorentz considered a gas of N particles. The applied electric field $\mathbf{E}_0$ polarizes this gas so that the electric field $\mathbf{E}$ inside has a mean value given by $\mathbf{E}_0 = (1+\chi)\langle\mathbf{E}\rangle$, where $\langle\mathbf{E}\rangle$ denotes the field averaged over particle configurations. We consider a conceptual correspondence; the applied field corresponds to the bare line, the mean internal field to the dressed line.

The internal field at point $\mathbf{r}$ is a sum of the applied field and polarization fields of individual particles, $\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + \sum_{i=1}^{N}\mathbf{E}_i(\mathbf{r})$. The polarization field of particle i is $\mathbf{E}_i(\mathbf{r}) = M_i(\mathbf{r}-\mathbf{r}_i)\mathbf{E}^{(i)}(\mathbf{r}_i)$, determined by the field $\mathbf{E}^{(i)}(\mathbf{r}_i)$ acting on this particle and the tensor M_i describing its polarizability and propagation of the field.

It is customary to assume that the field acting on a particle is equal to the internal field, $\mathbf{E}^{(i)}(\mathbf{r}_i) \approx \mathbf{E}(\mathbf{r}_i)$. Such a step corresponds to the fully self-consistent approximation; the internal field is taken as the only physically relevant quantity in the system. However, the polarization field diverges in the dipole approximation, $\mathbf{E}^{(i)}(\mathbf{r}_i) \to \infty$. In the very dilute case one can remove the divergence using the applied field, $\mathbf{E}^{(i)}(\mathbf{r}_i) \approx \mathbf{E}_0(\mathbf{r}_i)$, and eventually add contributions of two, three, and more particles. This corresponds to the non-self-consistent expansion.

The mean field is also free of divergences; therefore, it is plausible to write $\mathbf{E}^{(i)}(\mathbf{r}_i) \approx \langle\mathbf{E}(\mathbf{r}_i)\rangle$ as a basis of a convergent fully self-consistent approximation. Such an approximation amounts to the use of an averaged field as a source in internal processes and cannot generally be justified. The correct procedure would be to evaluate the electric field for each configuration and to perform the average only as a final step.

The solution proposed by Lorentz is simple and elegant. Since the particle does not act on itself, it is correct to exclude its contribution, writing $\mathbf{E}^{(i)}(\mathbf{r}_i) = \mathbf{E}_0(\mathbf{r}_i) + \sum_{j\neq i}^{N}\mathbf{E}_j(\mathbf{r}_i)$. To close the set of equations one needs $\mathbf{E}^{(i)}$ as a function of the mean internal field. To this end surrounding particles are represented by the effective medium located everywhere except for the vicinity of the particle i. The field acting on the particle i is then the field inside a spherical cavity, $\mathbf{E}^{(i)}(\mathbf{r}_i) = \langle\mathbf{E}(\mathbf{r}_i)\rangle(1+\chi)/(1+\frac{2}{3}\chi)$. In this way Lorentz achieves self-consistency, avoiding the action of a given particle on itself.

One can adapt this Lorentz principle of self-consistency to the interacting Fermi liquid in two different ways. First, one can view fermions as Lorentz particles and their interaction as the internal field. The Lorentz self-consistency then eliminates self-interaction; this is discussed in Sec. III. The second approach is slightly more involved. The wave function of a selected particle plays the role of the electric field propagating in the medium, and is scattered by all other particles. This

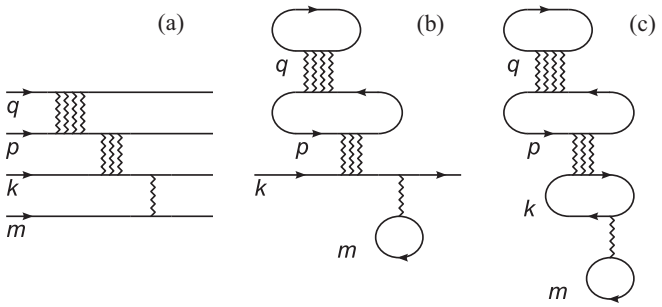

FIG. 1. Condensate-mediated self-interaction. Arrows represent bare fermionic Green's functions G_0 and wavy lines are boson-mediated interactions. (a) Schematic picture of four interacting particles of initial momenta k, p, q, and m. Due to the Pauli principle all particles are in different states, in particular $m \neq k$ and $q \neq k$, and $p \neq m$. (b),(c) Corresponding Feynman diagrams for the Green's function of the particle k and for the thermodynamical potential. For lines closed into loops momenta are summed over with no restriction.

approach, eliminating nonphysical repetition of collisions, is discussed in Sec. VI.

B. Self-interaction mediated by the condensate

A self-interaction can be of various types; here we focus on a self-interaction which is mediated by the condensate. Before we discuss this complex process, it is worthwhile to recall the simple self-interaction appearing in the familiar context of the mean field, when the true interaction is approximated by the scalar potential due to all electrons. In Figs. 1(b) and 1(c) one can see the lowest order of the mean-field potential given by the potential line and loop of summation index m.

The relative error due to the mean-field self-interaction depends on the size of the system. In a single atom, each electron is bounded by a potential which asymptotically approaches the Coulomb potential of the remaining ion. In the mean-field approximation, however, the atom is neutral and the binding potential asymptotically approaches zero. In the infinite system with delocalized electrons the self-interaction is negligible. It becomes essential, however, when the infinite system contains bound states.

The mean-field self-interaction cancels with a corresponding "self-exchange" of the Fock term. For details, see Appendix A . Although it is understood that eventually, due to higher-order diagrams, all self-interactions will compensate each other and the correct theory will emerge, such a formulation is not viable for practical approximations. We see in the next section that it is far more profitable to reconsider the summation rule itself and to exclude the self-interaction directly as it is done in the original theory of Hartree.

A self-interaction mediated by the condensate is shown in Fig. 1. The summation procedure does not respect that $m \neq k$, yielding the Hartree self-interaction at $m = k$. Now let us focus on the two-loop contribution in the upper part, which contains a more subtle self-interaction. We assume that $p \neq k$, which is always guaranteed for separable potentials of BCS type coupling only spin $\uparrow$ with spin $\downarrow$. Aside from their mutual interaction, particles p and k also interact with the other particles in the system. One such background particle is q, and the sum over q does not respect the condition $q \neq k$, leading to a self-interaction mediated by particle p. In the normal metal such mediated processes are negligible, but in the superconductor the condensate leads to enhancement of binary interactions with $p = -k$ and $q = -p$. The weight of contributions with $q = k$ is thus finite, so that such mediated processes may no longer be ignored.

We note that the q-loop merely dresses the p line. Expansions based on dressed Green's functions do not include the diagram in Fig. 1(b); its contribution is hidden inside the self-consistent scheme. In the non-self-consistent expansion one can eventually avoid this problem by demanding $q \neq k$. This implies that the Green's function in the p-loop is not dressed by all processes; its value does not include interaction with the state k. It thus becomes manifest that in the self-consistent expansion we need some concept of restricted self-consistency.

C. Repeated collisions

Figure 1 includes two sequential interactions of particle k with particles p and m. Since the T matrix describes the binary collision between k and p to infinite order, in the subsequent collision the particle k must actually encounter a different, new partner. However, expanding the dressed Green's function in powers of the self-energy $G = G_0 + G_0\Sigma G_0 + G_0\Sigma G_0\Sigma G_0 + \cdots$, one can see that sequential events are described by successive products of the self-energy Σ. By definition, the self-energy includes all processes and there is no restriction with respect to the previous Σ factor.

Mediated self-interactions and repeated collisions are closely connected concepts. Figure 1(c) shows the diagram for the thermodynamic potential from which one can generate the diagram of Fig. 1(b). The contribution with $p = m$ can be classified either as a self-interaction mediated by particle k, or as a repeated collision along the propagation line of particle k. Similarly, $q = k$ is either a mediated self-interaction or a repeated collision on the p line. We shall indeed find that a restriction of mediated self-interaction is in fact equivalent to an elimination of repeated nonphysical collisions.

D. Dichotomy of self-consistency and gap

In self-consistent approximations the self-energy $\Sigma[G]$ is a functional of the dressed Green's function G. The T matrix $T \sim \delta\Sigma/\delta G$ becomes divergent below the critical temperature in the pairing channel; this is the element connecting a particle of energy, momentum, and spin $k = (\omega,\mathbf{k},\uparrow)$ with its conjugate $-k = (-\omega,-\mathbf{k},\downarrow)$. Keeping the divergent term only, $\Sigma(k) \approx T^{\mathrm{div}}G(-k)$, the Dyson equation $G = G_0 + G_0\Sigma G$ is easily solved, giving $G = (1 - \sqrt{1 - 4T^{\mathrm{div}}/(\omega^2 - \xi_k^2)})(\omega + \xi_k)/(2T^{\mathrm{div}})$. This peculiar dressed Green's function exhibits no gap. In the bare Green's function $G_0^{-1} = \omega - \xi_k$ we have used a symmetric band structure $\xi_{-k} = \xi_k = k^2/2m - \mu$ for simplicity.

The gap easily emerges in the non-self-consistent approximation $\Sigma[G_0]$ with the T matrix $T_0 \sim \delta\Sigma/\delta G_0$. Keeping the divergent term, $\Sigma(k) \approx T_0^{\mathrm{div}}G_0(-k)$, the Dyson equation results in the Gor'kov Green's function $G^{-1} = \omega - \xi_k - T_0^{\mathrm{div}}/(-\omega - \xi_k)$ with two poles at $\omega = \pm\sqrt{\xi_k^2 - T_0^{\mathrm{div}}}$. The

divergent element of the T matrix is a separable function which splits into products of two gap functions $T_0^{\mathrm{div}} = -\Delta^*\Delta$.

The fundamental problems of the self-consistent approximation stem from the scale dependence of the Brillouin-Wigner self-consistent expansion scheme, while the non-self-consistent perturbative expansion of Rayleigh-Schrödinger type is size-consistent.[46] As already mentioned, approximations which produce errors for few-body systems do so also in the superconducting state because of condensate-assisted processes.

The gap is a necessary part of any theory of superconductivity. The self-consistency is required only in some situations, for example, the Thouless criterion of the superconducting transition, or by the closely related existence of a Goldstone mode.[26] What is less well known is that the missing self-consistency also causes trouble in microscopic studies of nonequilibrium superconductivity beyond linear response. At some stage any study reaches the problem of a "non-self-consistent" distribution which is most commonly circumvented by an (often implicit) assumption of local equilibrium.

E. Galitskii-Feynman versus Kadanoff-Martin

The GF and the KM approximations are compared in diagrammatic representation in Fig. 2. Both are based on the many-body T matrix in the ladder approximation. As one can see, the KM approximation is nothing more than a simplified version of the GF approximation, neglecting an exchange and possessing only a bare line in the closed loop of self-energy, and in fact the exchange channel contributes only if the particles have parallel spins. Nevertheless, these two approximations are quite different with disjunct fields of application.

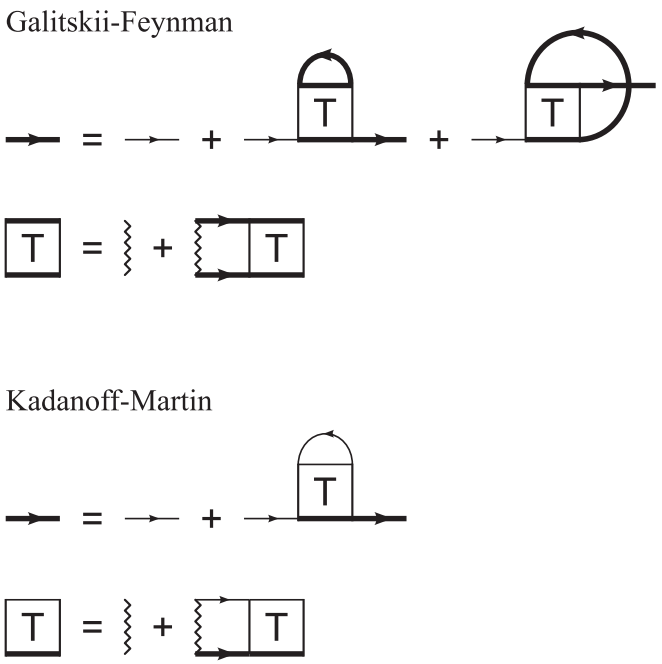

FIG. 2. T-matrix approximations in diagrams. Both approximations have a self-energy constructed from the many-body T matrix. The interaction carried by boson propagators, shown by wavy lines, is included in the ladder approximation. Thick arrows are self-energy dressed Green's functions, while thin arrows are bare Green's functions.

The GF approximation is used in nuclear physics for both equilibrium[47–49] and nonequilibrium[50,51] problems, in the theory of moderately dense gases[52] and liquid He-III (Ref. 53), and in studies of electron-electron correlations in molecules and solids.[54–58] There exist several reasons why the KM approximation was never adapted to these problems. The most important one is that the conservation laws are guaranteed only if the T matrix is symmetric with respect to the interchange of the upper and the lower line of the intermediate propagators;[41] thus, the lack of symmetry in the KM approximation is viewed as unjustified and unacceptable.

The KM approximation is used exclusively in the theory of superconductivity.[21,23,59–66] It describes the superconducting gap on the level of mean-field theory and covers the lowest-order fluctuations. The GF approximation cannot be employed for superconductors in spite of its superiority in other fields. Although it becomes unstable at the critical temperature[67] and the T matrix diverges there, the GF self-energy constructed from the T matrix fails to describe the superconducting gap.[19,68] This is the general problem of self-consistent theories discussed in the previous section.

The paradox that the worse approximation (KM) yields the gap while the better one (GF) fails in this regard was first noticed by Prange[69] and confirmed by Wild,[68] prior to the work of Kadanoff and Martin.[19] The Prange paradox[70] is not common knowledge and some authors (see, e.g., Ref. 71) report a superconducting gap obtained within the GF approximation. Upon closer inspection one finds that in simplification of some formulas, the bare Green's function is used to close loops,[22] a step which, in fact, turns the GF into the KM approximation.

F. Thouless criterion

The connection between formal perturbation theory and BCS-type theories has been discussed by Thouless.[72] It was found that when the phase transition is approached from above, the critical temperature can be determined through a criterion of stability of the normal state; a divergence of the two-particle T-matrix signals the transition. Thouless evaluated the T matrix from non-self-consistent Green's functions, but mentioned that corrections to the single-particle functions are desirable.

The Thouless criterion also follows from Goldstone's theorem.[26] The superconducting state is degenerate with respect to the complex phase of the gap. According to Goldstone's theorem, there must be a corresponding branch of collective excitations with energy going to zero in the long-wavelength limit. The gap appears as a divergence of the T matrix at the frequency and momentum of this Goldstone mode. For a constant complex phase, this divergence is at zero frequency and momentum. At the critical temperature the divergence gives the Thouless criterion for the nucleation of superconductivity. The variational nature of this approach demands that all Green's functions in the T matrix be self-consistent.[26]

True self-consistency is essential. Beach, Gooding, and Marsiglio compared the self-consistent Thouless criterion with its non-self-consistent approximation in the attractive Hubbard

model.[22] They report that the non-self-consistent criterion yields a finite critical temperature while the self-consistent one predicts a zero-temperature transition. Following recent common use, by "Thouless criterion" we always mean its fully self-consistent form.

When formulated via the response to the complex phase modulation as above, satisfaction of the Thouless criterion may be considered a transport problem. Any system away from equilibrium requires self-consistent distributions; the non-self-consistent functions can be used only under the assumption of local equilibrium, by which one typically loses control over neglected terms. As an example we mention the normal-current contribution to the time-dependent Ginzburg-Landau equation, derived from the Thouless criterion[73] and shown to contribute already at the level of linear response.[74]

It seems that neither the fully self-consistent nor the partly non-self-consistent diagrammatic approach can satisfy essential theoretical criteria for a fundamental theory of superconductivity. In the following section we introduce the RSC theory and begin to show how restricted self-consistency solves this problem.

III. ELIMINATED SELF-INTERACTIONS

We derive here a complete set of equations describing superconductivity, which constitute the RSC theory. This is done via an intuitive approach involving simple removal of the self-interaction mediated by the condensate, thus allowing formation of the gap.

A. Restricted self-energy

When two particles interact, their total energy and momentum $Q \equiv (\Omega, \mathbf{Q})$ is conserved; we may use this Q to label binary processes. Dressing of a particle of four-momentum k is given by the self-energy $\Sigma_\uparrow(k)$, which is a sum over interacting pairs,

$$\Sigma_\uparrow(k) = \sum_Q \left(\sigma_{Q\uparrow}(k) + \sigma^{\mathrm{trp}}_{Q\uparrow}(k) + \sigma^{\mathrm{exg}}_{Q\uparrow}(k)\right). \tag{1}$$

Here $\sigma_{Q\uparrow}(k)$ is a singlet contribution of single Q and $\sum_Q \cdots \equiv \sum_\Omega \sum_{\mathbf{Q}} \cdots$ denotes sums over bosonic Matsubara frequencies and discrete momenta in the quantization volume V. Function $\sigma^{\mathrm{trp}}_{Q\uparrow}(k)$ is a triplet contribution and $\sigma^{\mathrm{exg}}_{Q\uparrow}(k)$ is its exchange counterpart. We assume singlet pairing and explicitly treat only the singlet term.

The self-energy represents binary interactions averaged over all possible many-body wave functions. This corresponds to the susceptibility in the Lorentz problem. Now we focus on the binary interaction in which the total four-momentum is Q. All other processes are treated as a background, represented by a sum,

$$\Sigma_{\overline{Q}\uparrow}(k) = \sum_{Q' \neq Q} \sigma_{Q'\uparrow}(k) + \sum_{Q'} \left(\sigma^{\mathrm{trp}}_{Q'\uparrow}(k) + \sigma^{\mathrm{exg}}_{Q'\uparrow}(k)\right), \tag{2}$$

over all modes but the Q mode. The corresponding RSC Green's function is

$$G_{\overline{Q}\uparrow}(k) = G^0_\uparrow(k) + G^0_\uparrow(k)\Sigma_{\overline{Q}\uparrow}(k)G_{\overline{Q}\uparrow}(k), \tag{3}$$

where $G^0_\uparrow$ is the bare Green's function.

In the spirit of the Lorentz approach we can also express the restricted self-energy via a "cavity" in the effective medium:

$$\Sigma_{\overline{Q}\uparrow}(k) = \Sigma_\uparrow(k) - \sigma_{Q\uparrow}(k). \tag{4}$$

Since the dressed Green's function is given by the Dyson equation,

$$G_\uparrow(k) = G^0_\uparrow(k) + G^0_\uparrow(k)\Sigma_\uparrow(k)G_\uparrow(k), \tag{5}$$

we can express the RSC Green's function via the dressed one,

$$G_{\overline{Q}\uparrow}(k) = G_\uparrow(k) - G_\uparrow(k)\sigma_{Q\uparrow}(k)G_{\overline{Q}\uparrow}(k). \tag{6}$$

This will allow us to close the self-consistency for the dressed Green's function avoiding the self-interaction and problems with the gap.

For the sake of clarity, we have written equations for only a selected spin orientation; the complementary equations are obtained simply by flipping all spins.

B. T matrix

The contribution of the Q mode to the self-energy reads

$$\sigma_{Q\uparrow}(k) = \frac{k_B T}{V}\mathcal{T}_{\uparrow\downarrow}(k, Q-k; k, Q-k)G_{\overline{Q}\downarrow}(Q-k), \tag{7}$$

and similarly,

$$\sigma^{\mathrm{trp}}_{Q\uparrow}(k) = \frac{k_B T}{V}\mathcal{T}_{\uparrow\uparrow}(k, Q-k; k, Q-k)G_\uparrow(Q-k). \tag{8}$$

The exchange channel reads

$$\sigma^{\mathrm{exg}}_{Q\uparrow}(k) = \frac{k_B T}{V}\mathcal{T}_{\uparrow\uparrow}(k, Q-k; Q-k, k)G_\uparrow(Q-k). \tag{9}$$

We have used the RSC Green's function $G_{\overline{Q}\downarrow}(Q-k)$ to close the loop of the singlet channel (7). In this way we have eliminated the interaction of the $(Q-k;\downarrow)$ particle with the $(k;\uparrow)$ particle and therefore the mediated self-interaction of the $(k;\uparrow)$ particle.

To disallow self-interactions in intermediate processes the T matrix must be constructed as

$$\begin{aligned}\mathcal{T}_{\uparrow\downarrow}&(k, Q-k; p, Q-p) \\ &= D(k, Q-k; p, Q-p) - \frac{k_B T}{V}\sum_{k'} D(k, Q-k; k', Q-k') \\ &\quad \times G_\uparrow(k')G_{\overline{Q}\downarrow}(Q-k')\mathcal{T}_{\uparrow\downarrow}(k', Q-k'; p, Q-p),\end{aligned} \tag{10}$$

where D is a bosonic interaction line with interaction vertices included. The sum runs over momenta and fermionic Matsubara frequencies. We follow the sign convention of Ref. 75, Sec. 14.2, with D becoming the interaction potential in the nonretarded limit. The triplet T matrix $\mathcal{T}_{\uparrow\uparrow}$ is analogous, with both Green's functions dressed,

$$\begin{aligned}\mathcal{T}_{\uparrow\uparrow}&(k, Q-k; p, Q-p) \\ &= D(k, Q-k; p, Q-p) - \frac{k_B T}{V}\sum_{k'} D(k, Q-k; k', Q-k') \\ &\quad \times G_\uparrow(k')G_\uparrow(Q-k')\mathcal{T}_{\uparrow\uparrow}(k', Q-k'; p, Q-p).\end{aligned} \tag{11}$$

The set of equations is closed by the relation for the density of particles,

$$n_\uparrow = \frac{k_B T}{V} \sum_k G_\uparrow(k) e^{-i\omega\eta}, \tag{12}$$

with η infinitesimal and positive. This relation determines the chemical potential; in equilibrium metals the electrons of spin $\uparrow$ and $\downarrow$ have identical chemical potential, but in transient systems two different chemical potentials might be defined by this relation.

The set (1)–(12) constitutes the RSC theory. This is the main result of the present paper, and provides a complete description of superconductivity. We will return to its derivation later in Sec. VI. We take a moment to remind the reader that while this set of equations describing the RSC theory can be represented diagrammatically, it must be remembered that the usual Feynman rules have been modified.

IV. GAP AND SELF-CONSISTENCY

We now endeavor to show that the RSC theory constructed in the preceding section not only yields the gap, but also satisfies the Thouless criterion. We then prove that it exhibits the two-particle symmetries which are the Baym and Kadanoff criteria for conserving theories.

A. Gap equation

In the superconducting state there is a singlet channel in which the T matrix becomes singular. In equilibrium this divergence appears at zero energy, $\Omega = 0$, and in the absence of currents it is at zero momentum, $\mathbf{Q} = \mathbf{0}$. This is the mode $Q = 0 \equiv (0,\mathbf{0})$. Its T matrix is separable[44,67] and diverges proportional to the volume so that this single-mode contribution to the sum is finite in the limits $V \to \infty$ and $T \to 0$:

$$\frac{k_B T}{V} \mathcal{T}_{\uparrow\downarrow}(k, -k; p, -p) = -\phi^*(k)\phi(p). \tag{13}$$

The zero-mode contribution to the self-energy has a finite value,

$$\sigma_{0\uparrow}(k) = -\phi^*(k) G_{\bar{0}\uparrow}(-k)\phi(k). \tag{14}$$

According to (4), the self-energy is a sum of the zero-mode contribution and the restricted self-energy,

$$\Sigma_\uparrow(k) = -\phi^*(k) G_{\bar{0}\uparrow}(-k)\phi(k) + \Sigma_{\bar{0}\uparrow}(k). \tag{15}$$

The singularity thus does not enter the RSC Green's function $G_{\bar{0}\uparrow}$. One can consider $G_{\bar{0}\uparrow}$ as the Green's function of the normal metal.

Using (6), the dressed Green's function can be expressed via the RSC propagator

$$G_\uparrow(k) = G_{\bar{0}\uparrow}(k) - G_{\bar{0}\uparrow}(k)\phi^*(k) G_{\bar{0}\downarrow}(-k)\phi(k) G_\uparrow(k). \tag{16}$$

This equation shows that $\phi(k)$ equals the energy- and momentum-dependent anomalous self-energy, which gives the superconducting gap.

To connect with the Eliashberg theory we assume the system to be symmetric in spins, $G^0_\downarrow(k) = G^0_\uparrow(k)$, and have no supercurrent so that $G^0_\uparrow(\omega, -\mathbf{k}) = G^0_\uparrow(\omega,\mathbf{k})$. Splitting the restricted self-energy into its even and odd parts,

$$\chi(k) = \frac{1}{2}(\Sigma_{\bar{0}\uparrow}(k) + \Sigma_{\bar{0}\downarrow}(-k)), \tag{17}$$

$$\omega(Z(k) - 1) = \frac{1}{2}(\Sigma_{\bar{0}\uparrow}(k) - \Sigma_{\bar{0}\downarrow}(-k)), \tag{18}$$

one can express Eq. (16) as

$$\begin{aligned} G^{-1}_\uparrow(k) &= \omega - \xi_{\mathbf{k}} - \Sigma_{\bar{0}\uparrow}(k) + \frac{\phi^*(k)\phi(k)}{-\omega - \xi_{\mathbf{k}} - \Sigma_{\bar{0}\downarrow}(-k)} \\ &= \omega Z(k) - \xi_{\mathbf{k}} - \chi(k) + \frac{\phi^*(k)\phi(k)}{-\omega Z(k) - \xi_{\mathbf{k}} - \chi(k)}. \end{aligned} \tag{19}$$

The gap in energy spectrum is sharp for real $\chi(k)$, when it has the renormalization familiar from the Eliashberg theory,[1]

$$\Delta(k) = \frac{\phi(k)}{Z(k)}. \tag{20}$$

The anomalous self-energy itself follows from the equation for the T matrix (10) and the separability (13),

$$\begin{aligned} \phi^*(k) = -\frac{k_B T}{V} \sum_{k'} & D(k, -k; k', -k') \\ & \times G_\uparrow(k') G_{\bar{0}\downarrow}(-k')\phi^*(k'). \end{aligned} \tag{21}$$

Deriving (21) we have used that $D/V \to 0$ in the thermodynamic limit. This gap equation is a modified Eliashberg equation for the off-diagonal self-energy.[76]

At the critical line the gap vanishes and the nucleation kernel approaches the normal state value, $DGG_{\bar{0}} \to DGG$. Here we thus obtain the T matrix made of fully self-consistent Green's functions. We show that the RSC theory coincides with the GF theory in the normal state of an infinite system. That it satisfies the Thouless criterion discussed in Sec. II F is then a direct consequence of this general limit.

In the normal state, the T matrix has a finite value, $\mathcal{T} \sim D$. According to (7) the single-mode contribution to the self-energy vanishes in the thermodynamic limit, $\sigma_{Q\uparrow} \propto 1/V \to 0$. The RSC Green's function in this case is equal to the dressed Green's function, $G_{\bar{Q}\uparrow} \to G_\uparrow$, and the RSC theory may be identified with the GF approximation.

B. Eliashberg equation

The Eliashberg equation is a simple approximation of the present RSC theory: The reduced self-energy is approximated by the Migdal self-energy,

$$\begin{aligned} \Sigma_{\bar{0}\downarrow}(k) &\approx \Sigma^{\mathrm{M}}_\downarrow(k) \\ &= \frac{k_B T}{V} \sum_Q D(k, Q-k; Q-k, k) G_\uparrow(Q-k). \end{aligned} \tag{22}$$

The Migdal self-energy is included in the T matrix as its first-order approximation, $\mathcal{T} \approx D$, of the exchange channel; one may compare the summation in (22) with expression (9). It is easy to inlcude the singlet and direct-triplet channel at first order since they yield the mean field of Hartree type. This contribution is usually ignored for the phonon-mediated interaction, however.

We see that in the superconducting state the RSC theory closely parallels the Eliashberg theory, albeit with some differences. In the RSC theory all processes, whether they be normal collisions or Cooper pairing, are treated within the same T-matrix approximation. In the Eliashberg theory the normal processes are in the Migdal approximation while the pairing is covered by equations for the ϕ which is described by the approximation corresponding to the T matrix.

V. TWO-PARTICLE SYMMETRY AND CONSERVATION LAWS

In this section we demonstrate that the RSC theory satisfies symmetry conditions formulated by Baym and Kadanoff[41] as necessary for any theory to be conserving. It is important to qualify this by noting that these conditions alone are not sufficient; it cannot thereby be claimed that the theory is conserving in the Baym-Kadanoff sense, since the symmetries are actually required to obtain *in general*, while our RSC theory is limited to *equilibrium*.

A. Baym-Kadanoff conditions

Let us rewrite both conditions of Baym and Kadanoff in the present notation. The first BK condition states that the self-energy is linked to the two-particle Green's function $\mathcal{G}$ in two equivalent ways,

$$\begin{aligned}&\Sigma_\uparrow(k)G_\uparrow(k)\\&\quad=\left(\frac{k_BT}{V}\right)^2\sum_{Q,p}D(k,Q-k;p,Q-p)[\mathcal{G}_{\uparrow\uparrow}(p,Q\\&\qquad-p;k,Q-k)+\mathcal{G}_{\uparrow\downarrow}(p,Q-p;k,Q-k)],\end{aligned}\tag{23}$$

$$\begin{aligned}&G_\uparrow(k)\Sigma_\uparrow(k)\\&\quad=\left(\frac{k_BT}{V}\right)^2\sum_{Q,p}D(p,Q-p;k,Q-k)[\mathcal{G}_{\uparrow\uparrow}(k,Q\\&\qquad-k;p,Q-p)+\mathcal{G}_{\uparrow\downarrow}(k,Q-k;p,Q-p)].\end{aligned}\tag{24}$$

The second BK condition demands that the two-particle Green's function be symmetric with respect to the interchange of the upper and lower lines:

$$\mathcal{G}_{\uparrow\uparrow}(k,Q-k;p,Q-p)=\mathcal{G}_{\uparrow\uparrow}(Q-k,k;Q-p,p),\tag{25}$$

$$\mathcal{G}_{\uparrow\downarrow}(k,Q-k;p,Q-p)=\mathcal{G}_{\downarrow\uparrow}(Q-k,k;Q-p,p).\tag{26}$$

Though conditions (23)–(26) provide in the equilibrium case only limited indication of the validity of full conservation laws, it is significant that the RSC theory passes this test; one can easily show that the other theories we have mentioned fail to satisfy the BK conditions even in equilibrium. For example, the KM approximation does not satisfy the Baym-Kadanoff criterion (26). It should be noted that the precursor of the present RSC theory in Ref. 38 also fails to satisfy the symmetry in (26).

B. Two-particle Green's function

The self-energy can be split into triplet and singlet channels, and the symmetries for each contribution tested separately. The GF approximation satisfies both Baym-Kadanoff conditions.[41] The triplet channel in our theory is the same as in the GF theory and therefore satisfies (23), (24), and (25). We thus focus on the singlet channel in which the RSC theory differs from the GF approximation.

The condition (23) and (24) links the single-particle Green's function G with the two-particle function $\mathcal{G}$. In the present approximation the two-particle function is related to the T-matrix through

$$\begin{aligned}&\mathcal{G}_{\uparrow\downarrow}(k,Q-k;p,Q-p)\\&\quad=G_\uparrow(k)G_{\overline{Q}\downarrow}(Q-k)\delta(k-p)-G_\uparrow(k)G_{\overline{Q}\downarrow}(Q-k)\\&\qquad\times G_\uparrow(p)G_{\overline{Q}\downarrow}(Q-p)\mathcal{T}_{\uparrow\downarrow}(k,Q-k;p,Q-p).\end{aligned}\tag{27}$$

Substituting (27) into (23) and (24) one may check that both formulas yield the singlet self-energy given by relations (1), (7), and (10).

C. Two-particle symmetry

Condition (26) is somewhat nontrivial, demanding that the singlet two-particle function be invariant under interchange of the upper and lower lines. This symmetry is not obvious from expression (27).

First we show that the T matrix (10) is symmetric with respect to the interchange of the upper and lower lines

$$\mathcal{T}_{\uparrow\downarrow}(k,Q-k;p,Q-p)=\mathcal{T}_{\downarrow\uparrow}(Q-k,k;Q-p,p),\tag{28}$$

in spite of the fact that the upper line is constructed from RSC Green's functions while the lower line uses dressed Green's functions.

The T matrix is a functional of the interaction $\mathcal{T}[D]$, which can be expanded in powers. We prove the symmetry (28) to a general order n. First, we link powers of the T matrix with powers of the two-particle Green's function (27) using

$$\mathcal{T}_{\uparrow\downarrow}=D-\frac{V}{k_BT}\sum D\cdot\mathcal{G}_{\uparrow\downarrow}\cdot D,\tag{29}$$

which follows from (10) and (27). The T matrix to order n in powers of D thus depends on $\mathcal{G}$ to the power of $n-2$.

To prove the symmetry (28) we use induction. It is apparent that the symmetry (28) is satisfied for two lowest orders $\mathcal{T}^{(1)}=D$ and $\mathcal{T}^{(2)}=-D\mathcal{G}^{(0)}_{\uparrow\downarrow}D$, where $\mathcal{G}^{(0)}_{\uparrow\downarrow}=G^0G^0$. We assume that the T matrix is symmetric up to order $n-2$ and show that the order $n-2$ two-particle Green's function is then also symmetric. According to relation (29), this implies symmetry (28) to order n.

The Q-mode contribution to the self-energy (7) can be rearranged as

$$\begin{aligned}&\sigma_{Q\uparrow}(k)G_{\overline{Q}\uparrow}(k)\\&\quad=\frac{k_BT}{V}\mathcal{T}_{\uparrow\downarrow}(k,Q-k;k,Q-k)G_{\overline{Q}\downarrow}(Q-k)G_{\overline{Q}\uparrow}(k)\\&\quad=\frac{k_BT}{V}\mathcal{T}_{\downarrow\uparrow}(Q-k,k;Q-k,k)G_{\overline{Q}\downarrow}(Q-k)G_{\overline{Q}\uparrow}(k)\\&\quad=G_{\overline{Q}\downarrow}(Q-k)\sigma_{Q\downarrow}(Q-k).\end{aligned}\tag{30}$$

This relation is based on symmetry (28); therefore, it is justified to order $n-2$.

Using relation (30) we can rearrange the product of two single-particle Green's functions

$$\begin{aligned} &G_{\overline{Q}\uparrow}(k)G_{\downarrow}(Q-k) \\ &\quad = G_{\uparrow}(k)[1-\sigma_{Q\uparrow}(k)G_{\overline{Q}\uparrow}(k)] \\ &\qquad \times [1+G_{\downarrow}(Q-k)\sigma_{Q\downarrow}(Q-k)]G_{\overline{Q}\downarrow}(Q-k) \\ &\quad = G_{\uparrow}(k)G_{\overline{Q}\downarrow}(Q-k)[1-\sigma_{Q\downarrow}(Q-k)G_{\overline{Q}\downarrow}(Q-k)] \\ &\qquad \times [1+G_{\downarrow}(Q-k)\sigma_{Q\downarrow}(Q-k)] \\ &\quad = G_{\uparrow}(k)G_{\overline{Q}\downarrow}(Q-k). \end{aligned} \tag{31}$$

In the first step we have used (6) for Green's functions $G_{\downarrow}(Q-k)$ and $G_{\overline{Q}\uparrow}(k)$. In the second step we have substituted from Eq. (30). The last rearrangement follows again from (6).

Using the relation (31) in Eq. (27) one finds that from the symmetry of the T-matrix $\mathcal{T}$ follows the symmetry of the two-particle Green's function $\mathcal{G}$. We have thus proved that from the symmetry of $\mathcal{T}$ up to order $n-2$ follows the symmetry of $\mathcal{G}$ to the same order. Finally, using $\mathcal{G}$ symmetric up to order $n-2$, from Eq. (29) one finds that the T matrix is symmetric up to order n. We have thus proved the symmetry (28) to all orders.

From the symmetry of the T matrix follows the symmetry (26) of the two-particle Green's function. In equilibrium, the RSC theory thus satisfies the conditions of Baym and Kadanoff.

VI. MULTIPLE SCATTERING APPROACH

In the above derivation we have removed the self-interaction using the idea of Lorentz regarding the interaction potential. The theory can, in fact, be justified quite systematically using the Fadeev-Lovelace-Watson multiple scattering expansion[31–37] in which the Lorentz idea is applied to the wave function of a particle. One may note that while the multiple scattering theory approach in Ref. 38 was limited to nonretarded interactions, the following presentation is applicable to a general interaction mediated by bosons.

A. Coherent propagation

In the multiple scattering theory one assumes that it is possible to identify collisions of a selected particle. In the system of many identical particles this is obscured by the presence of exchange processes. Fortunately, we can trace the single-particle history in coherent propagation, which is essential for the formation of the gap.

Expanding the dressed Green's function (5) in powers of the self-energy, $G_{\uparrow}(k) = G^0_{\uparrow}(k) + G^0_{\uparrow}(k)\Sigma_{\uparrow}(k)G^0_{\uparrow}(k) + G^0_{\uparrow}(k)\Sigma_{\uparrow}(k)G^0_{\uparrow}(k)\Sigma_{\uparrow}(k)G^0_{\uparrow}(k) + \cdots$ one can see that between interactions an electron returns to its starting state $(k,\uparrow)$. The Dyson equation thus describes only coherent propagation.

In the Feynman expansion one can associate each self-energy contribution $\sigma_{Q\uparrow}(k)$ with an encounter of a particle in state $(k,\uparrow)$ with a particle in state $(Q-k,\downarrow)$. In coherent propagation both particles return to their initial states, as can be seen in the arguments of the T matrix in (7). Following Landau we call such encounters *zero-angle collisions*.

The product $G^0_{\uparrow}\Sigma_{\uparrow}G^0_{\uparrow}\Sigma_{\uparrow}G^0_{\uparrow}$ represents two subsequent zero-angle collisions. In the GF approximation such a product includes terms $G^0_{\uparrow}(k)\sigma_{Q\uparrow}(k)G^0_{\uparrow}(k)\sigma_{Q\uparrow}(k)G^0_{\uparrow}(k)$ in which the particle in the $(k;\uparrow)$ state encounters the particle in the $(Q-k;\downarrow)$ state. Since after the first encounter both particles returned to their initial states, the second self-energy thus describes an encounter of the same pair of particles. Such repeated zero-angle collision is, in fact, incompatible with the T matrix because its ladder approximation already covers the binary interaction to infinite order. Finite states of a completed collision given by the T matrix cannot serve as initial states for the same process again.

B. Effective medium

The repeated zero-angle collision is a double-count equivalent to the molecule polarized by its own radiation in the Lorentz problem and we can remove it with similar theoretical tools. Application of the Lorentz idea to fermions was put forward by Watson,[31,32] who formulated the perturbative expansion in terms of binary T matrices showing that repeated collision must be avoided. His multiple-scattering approach was further developed in two directions. Fadeev[33–35] and Lovelace[36] have worked with detailed applications to small systems. Soven[40,77,78] has applied the multiple-scattering approach to scattering of electrons on static random potential in alloys. We adopt Soven's concept of self-energy.

In parallel with the susceptibility, the self-energy can be viewed as an auxiliary complex potential which represents the mean effect of true collisions. Thus, instead of adding progressively more diagrams we look for a condition which determines the self-energy from a physical rather than mathematical viewpoint.

We focus on the $(k;\uparrow)$ particle making a zero-angle collision in the Q mode. Briefly, we want to evaluate the self-energy contribution $\sigma_{Q\uparrow}$. This process is described in detail by the T matrix $\mathcal{T}_{\uparrow\downarrow}(k,Q-k;k,Q-k)$. All other processes form an environment in which this one happens and are thus covered on the level of effective medium. In the spirit of Lorentz cavity we subtract the contribution $\sigma_{Q\uparrow}$ from the self-energy. The effective medium is thus described by the restricted self-energy $\Sigma_{\overline{Q}\uparrow}$ for the $\uparrow$ component and by the complete self-energy $\Sigma_{\downarrow}$ for the $\downarrow$ component.

The T matrix describes an interaction of two particles to infinite order. Since we focus on the $(k;\uparrow)$ particle, we have to average over the probability to find a collision partner in the $(Q-k;\downarrow)$ state,

$$s_{Q\uparrow}(k) = \frac{k_{\mathrm{B}}T}{\Omega}\mathcal{T}_{\uparrow\downarrow}(k,Q-k;k,Q-k)G_{\downarrow}(Q-k). \tag{32}$$

The collision in the Q mode is not to be repeated; therefore,

$$G_{\uparrow}(k) = G_{\overline{Q}\uparrow}(k) + G_{\overline{Q}\uparrow}(k)s_{Q\uparrow}(k)G_{\overline{Q}\uparrow}(k). \tag{33}$$

The scattering equation (33) defines the self-energy indirectly. Comparing (33) with (6) we find that the Q mode contribution to the self-energy is given by

$$\frac{\sigma_{Q\uparrow}(k)}{1-\sigma_{Q\uparrow}(k)G_{\overline{Q}\uparrow}(k)} = s_{Q\uparrow}(k). \tag{34}$$

Finally we need the many-body T matrix. Since our background is described by $\Sigma_{\overline{Q}\uparrow}$ and $\Sigma_{\downarrow}$, the ladder approximation of the many-body T matrix

$$\begin{aligned}\mathcal{T}_{\uparrow\downarrow}(k,Q-k;p,Q-p)&\\ = D(k,Q-k;p,Q-p)-\frac{k_{\mathrm{B}}T}{\Omega}\sum_{k'}D(k,Q-k;k',Q-k')&\\ \times G_{\overline{Q}\uparrow}(k')G_{\downarrow}(Q-k')\mathcal{T}_{\uparrow\downarrow}(k',Q-k';p,Q-p)&\end{aligned}\tag{35}$$

is constructed from $G_{\overline{Q}\uparrow}$ and $G_{\downarrow}$. The set of equations (1)–(6), (8)–(9), (11), and (34)–(35) is closed.

C. Relation to the eliminated self-interaction

The set of equations (1)–(6), (8)–(9), (11), and (34)–(35) is, in fact, equivalent to the set of equations (1)–(11) which we derived intuitively earlier in the paper and which define the RSC theory. To see this, we use the symmetry (31) and readily rewrite (35) to obtain (10). The two definitions of the T matrix are thus equivalent.

It remains to show that the self-energy is identical. From Eq. (34) we find

$$\begin{aligned}\sigma_{Q\uparrow}(k)&=s_{Q\uparrow}(k)(1-\sigma_{Q\uparrow}(k)G_{\overline{Q}\uparrow}(k))\\ &=s_{Q\uparrow}(k)(1-\sigma_{Q\downarrow}(Q-k)G_{\overline{Q}\downarrow}(Q-k))\\ &=\frac{k_{\mathrm{B}}T}{\Omega}\mathcal{T}_{\uparrow\downarrow}(k,Q-k;k,Q-k)\\ &\quad\times G_{\downarrow}(Q-k)(1-\sigma_{Q\downarrow}(Q-k)G_{\overline{Q}\downarrow}(Q-k))\\ &=\frac{k_{\mathrm{B}}T}{\Omega}\mathcal{T}_{\uparrow\downarrow}(k,Q-k;k,Q-k)G_{\overline{Q}\downarrow}(Q-k);\end{aligned}\tag{36}$$

therefore, the expressions (34) and (7) yield the same self-energy. In the rearrangement we have used (30) and (32).

D. Comments on choice of restriction

Finally, we want to comment on the relation of the RSC theory to the derivation in Ref. 38. Here we identify the mode via energy and momentum $Q\equiv(\omega,\mathbf{Q})$. In Ref. 38 the mode was identified only via momentum $\mathbf{Q}$, which applies only to nonretarded interactions and leads to different results.

In particular, the identification of a mode via momentum does not provide a two-particle Green's function symmetric with respect to interchange of the upper and lower lines. The theory in Ref. 38 thus does not satisfy the condition (26) of Baym and Kadanoff and cannot be converted into a more convenient form with restricted self-consistent Green's functions in the closed loop.

Apparently, one can derive a theory with restricted self-consistency in the loop and the mode identified via momentum $\mathbf{Q}$ by elimination of mediated self-interactions in a manner similar to the one employed in Sec. III A. A set of equations obtained in this way is not identical to the theory in Ref. 38. Differences are minor, however. The two approaches become identical in the single-mode approximation leading to the same equation of BCS type.

The RSC theory is restricted to equilibrium. In contrast, the theory in Ref. 38 is based exclusively on double-time functions, which allows one to extend it to nonequilibrium systems using either Kadanoff-Baym or Keldysh machinery.

Extension of the present RSC theory cannot be achieved by a straightforward application of the Kadanoff-Baym method. This is because the Q-mode contribution $\sigma_{Q\uparrow}(k)$, depends on two four-momenta, bosonic $Q\equiv(\Omega,\mathbf{Q})$ and fermionic $k\equiv(\omega,k)$. Functions of two frequencies correspond to three-time functions which have six analytic parts in the nonequilibrium extension. This makes the putative nonequilibrium version prohibitively complicated.

VII. SUMMARY AND CONCLUSION

Self-consistent theories are unviable for superconductivity, as they cannot yield a superconducting gap. So-called non-self-consistent approaches produce a gap, but can be shown to be nonconserving, failing to satisfy the necessary Baym-Kadanoff conditions. Applying principles of the multiple-scattering theory to the T-matrix approximation, we have derived a theory which describes the superconducting gap, the structure of this theory being similar to a renormalized KM approximation, but sporting two major improvements. First, in the normal state the well-tested GF approximation is recovered. Since the GF T matrix depends on self-consistent propagators, the RSC theory satisfies the Thouless criterion. Second, the two-particle propagator is symmetric with respect to interchange of the two lines in its defining Feynman diagram. This symmetry allows the RSC theory to satisfy the Baym-Kadanoff requirements for a conserving theory. Finally, though the RSC theory may be approximated by the Eliashberg theory, it may be noted that due to the more elaborate self-consistency of the RSC theory, superconductivity conditions in strongly interacting systems are likely to be different from the Eliashberg theory.

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APPENDIX A: MEAN-FIELD SELF-INTERACTION AND HARTREE APPROXIMATION

This appendix follows the introductory part of Slater's paper[79] in which was simplified the Hartree-Fock method, constructing the basis of the local-density approximation. Two simplifications are adopted within this section. First, we assume a ground state of N particles described by a single many-body wave function. Second, the interaction potential is of the Coulomb type. The Hamiltonian is thus a sum of the single-particle part and the interaction, $H=\sum_i H^{(1)}(x_i)+\sum_{k<i}V(x_i-x_k)$.

A. Hartree equations

The Hartree equations are obtained by minimizing the energy on the class of separable wave functions of the form

$$W_{\rm H} = \int dx_1 \ldots dx_2 \bar{\psi}_1(x_1) \ldots \bar{\psi}_N(x_N) H \psi_N(x_N) \ldots \psi_1(x_1), \tag{A1}$$

where x_i are coordinates, and a summation over spins is understood. Varying the ψ functions in the Hartree energy (A1) one finds

$$E_i \psi_i(x) = H^{(1)} \psi_i(x) + \left[\sum_{k \neq i} \int dx' \bar{\psi}_k(x') \psi_k(x') V(x - x') \right] \psi_i(x). \tag{A2}$$

Since the particle does not interact with itself, the term with $k = i$ is excluded from the sum.

The mean potential

$$\phi(x) = \sum_k \int dx' \bar{\psi}_k(x') \psi_k(x') V(x - x') \tag{A3}$$

includes contributions from all electrons. The Hartree equations can be written in terms of the mean potential as

$$E_i \psi_i(x) = H^{(1)} \psi_i(x) + \phi(x) \psi_i(x) - \left[\int dx' \bar{\psi}_i(x') \psi_i(x') V(x - x') \right] \psi_i(x). \tag{A4}$$

Briefly, the Hartree approximation is given by the mean potential corrected by the self-interaction.

B. Hartree-Fock equations

The Hartree-Fock equations are obtained by minimizing the energy, on the class of antisymmetrized separable functions of the form

$$W_{\rm HF} = \frac{1}{N!} \int dx_1 \ldots dx_2 \times \begin{vmatrix} \bar{\psi}_N(x_N) \ldots \bar{\psi}_N(x_1) \\ \ldots\ldots\ldots\ldots \\ \bar{\psi}_1(x_N) \ldots \bar{\psi}_1(x_1) \end{vmatrix} H \begin{vmatrix} \psi_1(x_1) \ldots \psi_1(x_N) \\ \ldots\ldots\ldots\ldots \\ \psi_N(x_1) \ldots \psi_N(x_N) \end{vmatrix}. \tag{A5}$$

Unlike in Hartree's case, the ψ functions in in Slater's determinant may be assumed to be orthogonal without loss of generality.

Varying the ψ functions in the energy (A5) one finds

$$E_i \psi_i(x) = H^{(1)} \psi_i(x) + \phi(x) \psi_i(x) - \sum_k \left[\int dx' \bar{\psi}_k(x') \psi_i(x') V(x - x') \right] \psi_k(x). \tag{A6}$$

The last term is due to the exchange of particles and it is customary to refer to it as the Fock potential. In this spirit the mean potential ϕ is often called the Hartree potential.

Note that the Fock term includes a $k = i$ contribution, therefore the self-interaction of the mean potential ϕ cancels with the self-exchange.

The Fock term corresponds to a single-electron charge. This can be seen from an effective density,

$$n_{i,x}(x') = \sum_k \frac{\bar{\psi}_i(x) \bar{\psi}_k(x') \psi_k(x) \psi_i(x')}{\bar{\psi}_i(x) \psi_i(x)}, \tag{A7}$$

in terms of which the Hartree-Fock equations are reminiscent of the usual single-particle Schrödinger equation:

$$E_i \psi_i(x) = H^{(1)} \psi_i(x) + \phi(x) \psi_i(x) - \left[\int dx' n_{i,x}(x') V(x - x') \right] \psi_i(x). \tag{A8}$$

The effective density corresponds to a single particle,

$$\int dx' n_{i,x}(x') = 1, \tag{A9}$$

as one finds integrating and summing the right-hand side of (A7). From orthogonality of the ψ functions follows that only the term with $k = i$ contributes.

APPENDIX B: MODEL OF REDUCED INTERACTION

The BCS wave function

$$|\Psi_{\rm BCS}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} \psi^\dagger_{\mathbf{p}\uparrow} \psi^\dagger_{-\mathbf{p}\downarrow}) |0\rangle \tag{B1}$$

is known to be the exact ground state in the limit of infinite volume for the reduced interaction

$$\hat{D} = -\frac{\lambda}{V} \sum_{\mathbf{k},\mathbf{p}} \psi^\dagger_{\mathbf{p}\uparrow} \psi^\dagger_{-\mathbf{p}\downarrow} \zeta_{\mathbf{p}} \zeta_{\mathbf{k}} \psi_{-\mathbf{k}\downarrow} \psi_{\mathbf{k}\uparrow}; \tag{B2}$$

that is,

$$D_{\uparrow\downarrow}(k, Q - k; p, Q - p) = -\lambda\, \zeta_{\mathbf{k}} \zeta_{\mathbf{p}} \delta_{\mathbf{Q},\mathbf{0}}, \qquad D_{\uparrow\uparrow} = 0. \tag{B3}$$

The ζ factors are form factors; ζ can be either a simple cutoff, for example, $\zeta_{\mathbf{k}} = \theta(\omega_{\rm c} - |\xi_{\mathbf{k}}|)$, or a more involved function covering nontrivial gap symmetries. We test the present approximation against this exact result.

1. Anomalous functions

The BCS state implies mean-field approximation of the self-energy. We discuss all approximations in the time representation, in which the Green's function is the mean value of time-ordered product of field operators in different times,

$$G_\uparrow(t, \mathbf{k}) = -i \langle \Psi_{\rm BCS} | \mathsf{T} \psi_{\mathbf{k}\uparrow}(t) \psi^\dagger_{\mathbf{k}\uparrow}(0) | \Psi_{\rm BCS} \rangle \equiv -i \langle \psi_{\mathbf{k}\uparrow} \psi^{\dagger 0}_{\mathbf{k}\uparrow} \rangle. \tag{B4}$$

From $G_0^{-1} = i\partial_t - \xi_{\mathbf{k}}$ follows

$$G_0^{-1} G_\uparrow = \delta(t) + \langle [\hat{D}, \psi_{\mathbf{k}\uparrow}] \psi^{\dagger 0}_{\mathbf{k}\uparrow} \rangle = \delta(t) + \zeta_{\mathbf{k}} \frac{\lambda}{V} \sum_{\mathbf{p}} \zeta_{\mathbf{p}} \langle \psi^\dagger_{-\mathbf{k}\downarrow} \psi_{-\mathbf{p}\downarrow} \psi_{\mathbf{p}\uparrow} \psi^{\dagger 0}_{\mathbf{k}\uparrow} \rangle. \tag{B5}$$

The two-particle Green's function exactly satisfies the anomalous decoupling

$$\langle \psi^\dagger_{-\mathbf{k}\downarrow} \psi_{-\mathbf{p}\downarrow} \psi_{\mathbf{p}\uparrow} \psi^{\dagger 0}_{\mathbf{k}\uparrow} \rangle = \langle \psi^\dagger_{-\mathbf{k}\downarrow} \psi_{-\mathbf{p}\downarrow} \rangle \langle \psi_{\mathbf{p}\uparrow} \psi^{\dagger 0}_{\mathbf{k}\uparrow} \rangle + \langle \psi^\dagger_{-\mathbf{k}\downarrow} \psi^{\dagger 0}_{\mathbf{k}\uparrow} \rangle \langle \psi_{-\mathbf{p}\downarrow} \psi_{\mathbf{p}\uparrow} \rangle. \tag{B6}$$

This is easily proved using the Bogoliubov-Valutin transformation $\psi_{\mathbf{k}\uparrow} = u_{\mathbf{k}}\gamma_{\mathbf{k}} + v_{\mathbf{k}}\beta^{\dagger}_{\mathbf{k}}$, and $\psi_{-\mathbf{k}\downarrow} = u_{\mathbf{k}}\beta_{\mathbf{k}} - v_{\mathbf{k}}\gamma^{\dagger}_{\mathbf{k}}$, where β and γ are annihilation operators of excitations above the BCS state, $\beta_{\mathbf{k}}|\Psi_{\mathrm{BCS}}\rangle = 0$ and $\gamma_{\mathbf{k}}|\Psi_{\mathrm{BCS}}\rangle = 0$. Using the anticommutation relation $\gamma_{\mathbf{k}}\gamma^{\dagger}_{\mathbf{p}} + \gamma^{\dagger}_{\mathbf{p}}\gamma_{\mathbf{k}} = \delta_{\mathbf{k},\mathbf{p}}$ between operators at equal times, one finds that both sides of (B6) equal $-v_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{p}}u_{\mathbf{p}}(1-\delta_{\mathbf{k},\mathbf{p}})\langle\gamma_{\mathbf{k}}\gamma^{\dagger 0}_{\mathbf{k}}\rangle$.

By decoupling (B6) one readily converts the nonperturbative equation of motion (B5) into the mean-field equation of Gor'kov type. The mean-field approximation for anomalous functions thus yields an exact solution for the reduced interaction (B1).

Now we show that restricted self-consistency also yields the exact solution. To this end we compare our equation for the RSC T matrix with Gor'kov equations.

Let us first write down the self-energy following from the Gor'kov theory. The product of normal mean values is proportional to $\delta_{\mathbf{k},\mathbf{p}}$. In the limit of infinite volume the contribution of this term to the interaction term in (B5) vanishes as $1/V$ and only the product of anomalous functions survives,

$$G_0^{-1}G_{\uparrow} = \delta(t) + \zeta_{\mathbf{k}}\frac{\lambda}{V}\sum_{\mathbf{p}}\zeta_{\mathbf{p}}\langle\psi_{-\mathbf{p}\downarrow}\psi_{\mathbf{p}\uparrow}\rangle\langle\psi^{\dagger}_{-\mathbf{k}\downarrow}\psi^{\dagger 0}_{\mathbf{k}\uparrow}\rangle. \tag{B7}$$

We denote the anomalous Green's function,

$$F^*(t;\mathbf{k}) = \langle\psi^{\dagger}_{-\mathbf{k}\downarrow}\psi^{\dagger 0}_{\mathbf{k}\uparrow}\rangle, \tag{B8}$$

and the gap function,

$$\Delta_{\mathbf{k}} = \zeta_{\mathbf{k}}\frac{\lambda}{V}\sum_{\mathbf{p}}\zeta_{\mathbf{p}}\langle\psi_{-\mathbf{p}\downarrow}\psi_{\mathbf{p}\uparrow}\rangle, \tag{B9}$$

in terms of which Eq. (B7) reads

$$G_0^{-1}G_{\uparrow} = \delta(t) + \Delta_{\mathbf{k}}F^*. \tag{B10}$$

Derivation of the equation for F^* is similar to the above derivation of Eq. (B10). It gives

$$\tilde{G}_0^{-1}F^* = -\Delta^*_{\mathbf{k}}G_{\uparrow}, \tag{B11}$$

where $\tilde{G}_0^{-1} = -i\partial_t - \xi_{-\mathbf{k}}$. The singular term $\delta(t)$ does not appear, as creation operators anticommute. The Δ^* is obtained from

$$\Delta^*_{\mathbf{k}} = \zeta_{\mathbf{k}}\frac{\lambda}{V}\sum_{\mathbf{p}}\zeta_{\mathbf{p}}F^*_{\mathbf{p}}, \tag{B12}$$

which is the Hermitian conjugate of Eq. (B9). Substituting the solution of (B11) in (B10) we find

$$G_0^{-1}G_{\uparrow} = \delta(t) - \Delta_{\mathbf{k}}\tilde{G}^0_{\downarrow}\Delta^*_{\mathbf{k}}G_{\uparrow}. \tag{B13}$$

The Fourier transformation of Eq. (B13) in time reads

$$(\omega - \xi_{\mathbf{k}})\,G_{\uparrow} = 1 - \Delta_{\mathbf{k}}\,(-\omega - \xi_{-\mathbf{k}})^{-1}\,\Delta^*_{\mathbf{k}}G_{\uparrow}. \tag{B14}$$

The self-energy defined as $G^{-1}_{\uparrow} = \omega - \xi_{\mathbf{k}} - \Sigma_{\uparrow}$ can be expressed in terms of the gap function as

$$\Sigma_{\uparrow}(k) = -\Delta_{\mathbf{k}}G^0_{\downarrow}(-k)\Delta^*_{\mathbf{k}}, \tag{B15}$$

where $G^0_{\downarrow}(-k) = (-\omega - \xi_{-\mathbf{k}})^{-1}$. This self-energy yields the exact Green's function for the infinite system with reduced interaction.

Finally, we write down an explicit gap equation. Using the anomalous Green's function from (B11) in the gap equation (B12) one finds

$$\Delta^*_{\mathbf{k}} = -\lambda\zeta_{\mathbf{k}}\frac{k_{\mathrm{B}}T}{V}\sum_{\mathbf{p},\omega}\zeta_{\mathbf{p}}G^0_{\downarrow}(-\omega,-\mathbf{p})\Delta^*_{\mathbf{p}}G_{\uparrow}(\omega,\mathbf{p}). \tag{B16}$$

We have evaluated the equal-time Green's function F^* needed in the gap equation by summing over Matsubara frequencies.

C. Restricted self-consistent T matrix

We compare the self-energy (B15) and the gap equation (B16) with their counterparts derived from the restricted self-consistent T-matrix.

In treating the RSC T-matrix we do not benefit from anomalous decoupling, but evaluate the resulting self-energy directly from the above set of Eqs. (1)–(11) with the reduced interaction (B3).

In Eqs. (10) and (11) we must include the spin dependence of the interaction line. Substituting $D_{\uparrow\uparrow}$ for D in (11) we obtain that the triplet T matrix vanishes; $\mathcal{T}_{\uparrow\uparrow} = 0$. The triplet and exchange self-energies (8) and (9) are thus trivial, $\sigma^{\mathrm{trp}}_{Q\uparrow}(k) = 0$ and $\sigma^{\mathrm{exg}}_{Q\uparrow}(k) = 0$.

With $D = D_{\uparrow\downarrow}$ the ladder equation (10) yields a nonzero singlet T matrix only for $\mathbf{Q} = 0$. The self-energy is thus a sum over only Matsubara frequencies:

$$\Sigma_{\uparrow}(\omega,\mathbf{k}) = \frac{k_{\mathrm{B}}T}{V}\sum_{\Omega}\mathcal{T}_{\uparrow\downarrow}(\omega,\mathbf{k},\Omega-\omega,-\mathbf{k};\omega,\mathbf{k},\Omega-\omega,-\mathbf{k}) \times G_{\overline{Q}\downarrow}(\Omega-\omega,-\mathbf{k}). \tag{B17}$$

The restricted self-energy,

$$\Sigma_{\overline{0}\uparrow}(\omega,\mathbf{k}) = \frac{k_{\mathrm{B}}T}{V}\sum_{\Omega\neq 0}\mathcal{T}_{\uparrow\downarrow}(\omega,\mathbf{k},\Omega-\omega,-\mathbf{k};\omega,\mathbf{k},\Omega-\omega,-\mathbf{k}) \times G_{\overline{Q}\downarrow}(\Omega-\omega,-\mathbf{k}), \tag{B18}$$

has no singularity proportional to the volume and there is no sum over momenta; therefore, it vanishes in the limit of infinite volume $V\to\infty$,

$$\Sigma_{\overline{0}\uparrow}(\omega,\mathbf{k}) = 0. \tag{B19}$$

The contribution of the zero Matsubara frequency, $Q = 0 \equiv (0,\mathbf{0})$, is enhanced by singularity of Bose-Einstein statistics at condensates; therefore,

$$\Sigma_{\uparrow}(k) = \frac{k_{\mathrm{B}}T}{V}\mathcal{T}_{\uparrow\downarrow}(k,-k;k,-k)\,G_{\overline{0}\downarrow}(-k). \tag{B20}$$

Since the restricted self-energy is zero, the restricted self-consistent Green's function equals to the bare Green's function

$$G_{\overline{0}\downarrow}(-k) = G^0_{\downarrow}(-k). \tag{B21}$$

Writing the only nontrivial term as

$$\mathcal{T}_{\uparrow\downarrow}(k,-k;k,-k) = -\frac{V}{k_{\mathrm{B}}T}\Delta^*_{\mathbf{k}}\Delta_{\mathbf{k}}, \tag{B22}$$

one arrives at the Gor'kov self-energy (B15). We have used $\chi(k) = 0$ and $Z(k) = 1$ following from (B19) so that $\phi(k) = \Delta_{\mathbf{k}}$.

It remains to prove that $\Delta^*_{\mathbf{k}}$ defined via Eq. (B21) satisfies the BCS gap equation (B16). This directly follows from the gap equation (21) which for the potential (B2) reads

$$\Delta^*(k) = -\lambda\,\zeta_{\mathbf{k}}\frac{k_{\mathrm{B}}T}{V}\sum_{k'}\zeta_{\mathbf{k}'}G_{\uparrow}(k')G_{\bar{0}\downarrow}(-k')\Delta^*(k'). \quad \text{(B23)}$$

The gap function does not depend on the Matsubara frequency ω, with $k \equiv (\omega,\mathbf{k})$, since the interaction is not retarded so that χ is independent of ω. Accordingly, $\Delta^*(k) = \Delta^*_{\mathbf{k}}$. Denoting $k' \equiv (\omega',\mathbf{k}')$ and using Eq. (B21) one recovers the BCS gap equation (B16).

The restricted self-consistent T matrix thus also yields the exact result for this special model.

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