Equivalence of the channel-corrected-*T*-matrix and anomalous-propagator approaches to condensation

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Any many-body approximation corrected for unphysical repeated collisions in a given condensation channel is shown to provide the same set of equations as they appear by using anomalous propagators. The *ad hoc* assumption in the latter theory about nonconservation of particle numbers can be released. In this way, the widespread used anomalous-propagator approach is given another physical interpretation. A generalized Soven equation follows which improves a chosen approximation in the same way as the coherent-potential approximation improves the averaged *T* matrix for impurity scattering.

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Superconducting and Bose-Einstein condensation phenomena belong to one of the most exciting macroscopic effects based on microscopic quantum physics. The theoretical description of both phenomena is one of the major activities in theoretical many-body physics. Superconductivity is based on the pairing of two fermions which form a condensate while bosons provide a one-particle Bose-Einstein condensate. Both phenomena are characterized by possessing a singular channel in which the effect appears.

The self-consistent multiple scattering T matrix in a many-body surrounding diverges near the critical temperature of the onset of the symmetry-broken phase, may it be pairing condensation for fermions or Bose-Einstein condensation for bosons. Though describing correctly the onset of pairing, the T matrix does not provide the gap equation. This changes if an asymmetric breaking of the self-consistency in the T matrix is used, such that one of the two internal propagators is used self-consistently and the other nonself-consistently. Then the gap equation appears as the pole of the T matrix. This was observed by Kadanoff and Martin[1] and used later on[2–5], for early citations see Ref. 6. It has remained puzzling since a seemingly worse approximation leads to better results.

Recently it turned out that the repeated collisions with the same particle are responsible for this artifact.[4] Repeated collisions of two particles in the same state are unphysical since the particles move apart from each other after the collision. If these repeated collisions with the same state are removed from the T matrix, the correct gap equation appears and the condensate can be described without asymmetrical *ad hoc* assumptions about self-consistency. The advantage of eliminating only the contributions of single channels as proposed in Refs. 4 and 5 is that the formation of pairs and their condensation can be described within the same approximation. This has also resulted in the description of different phases in interacting Bose systems.[7] Formally such form can be derived by a systematic expansion of Feynman diagrams connecting different channels in the sense of cummulant expansion.[8]

On the other hand, there exist a well-established theory to describe systems with condensates in terms of anomalous functions, for review see Ref. 9. Let us consider bosonic particles which can form a condensate being either bosons or paired fermions. If the system processes a macroscopic number N_0 of such particles in the condensate represented by channel i, the expectation value of the creation operator a_0^+ of that state is very huge and to a good accuracy the creation operators $[a_0,a_0^+]\approx 0$ commute with each other as well as with all other states.[9] The number of particles is considered as nonconstant if the condensate is thought as a reservoir since scattering off and on the condensate may create/destroy pairs. Therefore the anomalous Green's function $G_{12}=\frac{1}{i}\langle Ta_{-k}a_k\rangle$ are nonzero besides the normal Green's function $G_{11}=\frac{1}{i}\langle Ta_k a_k^+\rangle$ describing the simultaneous excitation of a pair. This *ad hoc* assumption leads then to the description of the condensate and the gap equation for pairing. Please note that the nature of the condensate remains quite different whether it is composed of bosons or paired fermions.[10]

The question is now, how the two approaches above are related. In the first theory correcting the T matrix, we consider only microscopic correlations while the same result is obtained by the second approach where one assumes *ad hoc* from the beginning anomalous functions. In the second approach, the symmetry of the theory concerning particle conservation is obviously broken while in the first approach it remains conserving. So it seems to be worth to understand the relation between both approaches.

The aim of the present Brief Report is to show that indeed the first approach leads to the same structure of equations like the second one yielding expressions for the anomalous functions without assuming them. Indeed it will be shown that the theory is somehow overdetermined by the second approach in that one can work with half the number of equations if following the first procedure. In view of this, the virtue of the first approach consists in giving the anomalous function assumption a further microscopic meaning since they can be derived from theory.

Let us therefore shortly sketch the structure of the first approach. We split the self-energy into different channels, $\Sigma=\Sigma_j\Sigma_j$, where we assume for simplicity that we have only one singular channel i where the condensate appears. The unphysical multiple scatterings with the same channel are concerning a single channel and vanish in the thermodynamical limit. Therefore this deficiency does not matter in normal matter. If we have a singular channel due to the condensate, however, this correction becomes essential. We have to subtract this process, i.e., we define the subtracted propagator,

$$G_{\not i} = G - G_{\not i}\Sigma_i G \tag{1}$$

or $G^{-1}=G_{\not i}^{-1}-\Sigma_i$. Using the standard Dyson equation $G_0^{-1}=G^{-1}+\Sigma$, we obtain the relation

$$G_{\not i} = G_0 + G_0(\Sigma - \Sigma_i)G_{\not i} \tag{2}$$

which shows that in this propagator the own self-energy channel is subtracted, $\Sigma'=\Sigma-\Sigma_i$. Now we consider a general T matrix which represents the self-energy as $\Sigma'=\Sigma_{j\neq i}T_j\bar{G}$ where the channel T-matrix T_j as two-particle function is closed by an backward propagator $\bar{G}$. In the singular channel we subtract the repeated interaction within this channel. This is achieved by closing with the subtracted propagator $\Sigma_i=T_i\bar{G}_{\not i}$. Now we can rewrite the Dyson equation as

$$\begin{aligned} G^{-1} &= G_0^{-1} - \Sigma = G_0^{-1} - \Sigma' - \Sigma_i \\ &= G_0^{-1} - \Sigma' - T_i\bar{G}_{\not i} \\ &= G_0^{-1} - \Sigma' - T_i(\bar{G}_0^{-1} - \bar{\Sigma}')^{-1}, \end{aligned} \tag{3}$$

where in the last step we have used Eq. (2). Finally we rewrite Eq. (3) to obtain the full propagator in momentum-energy (Matsubara) representation $p=(\mathbf{p},\omega_n)$,

$$G(p) = \frac{\bar{G}_0^{-1}(p) - \bar{\Sigma}'(p)}{[G_0^{-1}(p) - \Sigma'(p)][\bar{G}_0^{-1}(p) - \bar{\Sigma}'(p)] - T_i(p)}. \tag{4}$$

Remembering $\Sigma'=\Sigma-T_i\bar{G}_{\not i}$ leads immediately back to the Dyson equation $G=G_0/(1-\Sigma G_0)$. Therefore it is an exact rewriting so far.

Now we take into account the explicit form of the free propagator $G_0^{-1}=\omega-\epsilon_k$ and $\bar{G}_0^{-1}=-\omega-\epsilon_{-k}$ and call the "proper" self-energy,

$$\Sigma_{11}(p) \equiv \Sigma'(p). \tag{5}$$

Further, we observe that the T matrix in the singular channel is separable[11–13] and can be written $T_i(p)=\pm\Delta(p)\bar{\Delta}(p)$ for bosons/fermions, respectively. Now we can define the "anomalous" self-energy as

$$\Sigma_{12}(p) \equiv \Delta(p) \tag{6}$$

such that the propagator [Eq. (4)] takes the form

$$G_{11} = \frac{\omega + \epsilon_{-k} + \bar{\Sigma}_{11}}{(\omega + \epsilon_{-k} + \bar{\Sigma}_{11})(\omega - \epsilon_k - \Sigma_{11}) \pm \Sigma_{12}^2}. \tag{7}$$

We add now an auxiliary quantity called anomalous Green's function

$$G_{12} \equiv \frac{\mp\Sigma_{12}}{(\omega + \epsilon_{-k} + \bar{\Sigma}_{11})(\omega - \epsilon_k - \Sigma_{11}) \pm \Sigma_{12}^2} \tag{8}$$

and can write in such a way the two equations in matrix form

$$\mathbf{G} = \mathbf{G^0} + \mathbf{G^0}\mathbf{\Sigma}\mathbf{G} \tag{9}$$

with

$$\mathbf{G} = \begin{pmatrix} G_{11} & G_{12} \\ \bar{G}_{12} & \pm\bar{G}_{11} \end{pmatrix}, \quad \mathbf{G}_0 = \begin{pmatrix} G_0 & 0 \\ 0 & \pm\bar{G}_0 \end{pmatrix},$$

$$\mathbf{\Sigma} = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \bar{\Sigma}_{12} & \pm\bar{\Sigma}_{11} \end{pmatrix} \tag{10}$$

for bosons/fermions, respectively. These are exactly the equations for anomalous propagators derived by Beliaev[14] for bosons. For fermions, these are the Nambu-Gorkov equations.[15]

In other words, separating a singular channel from the self-energy avoiding repeated collision within this channel leads immediately to propagators which have the Beliaev form for bosons or the Nambu-Gorkov form for fermions. We see that adding the auxiliary quantity [Eq. (8)] is not necessary. All information we have derived without this quantity and it was added here simply to show that the same structure of theory appears as provided by the approaches with anomalous functions. In this sense the theory of anomalous functions is overdetermined. We should note, however, that the anomalous propagator G_{12} describes the order parameter. This anomalous propagator appears as a result of the theory here and is not assumed from the beginning as done usually.

Now that we have clarified that the anomalous propagator is an exact rewriting of the Dyson equation if one correct a channel of self-energy for repeated collisions, we might ask what kind of equation such channel-corrected self-energy obeys. This will lead us to a generalization of the Soven equation.[16] The Soven equation was proposed to describe impurity scattering in terms of an effective medium and resulted in the coherent-potential approximation (CPA).[17–19] This CPA improves the averaged T matrix[20] with respect to better analytic properties and a wider range of applications. It has turned out that the averaged T matrix is the uncorrected channel while the CPA is equivalent to the channel-corrected approximation. Here we will present the same idea of channel correction but applied to the two-particle scattering. This will lead to a general Soven equation which allows to improve a chosen approximation scheme in the same manner as the CPA improves the averaged T-matrix approximation for impurity scattering.

Let s assume in general the defining equation for the channel T matrix in terms of the potential V and a block K_j,

$$T_j = V + VK_jT_j \tag{11}$$

covering both the singular channel $j=i$ as well as the normal channels $j\neq i$. In general this equation is a two-particle one which is reduced to the one-particle self-energy by closing the upper line with the backward propagating Green's func-

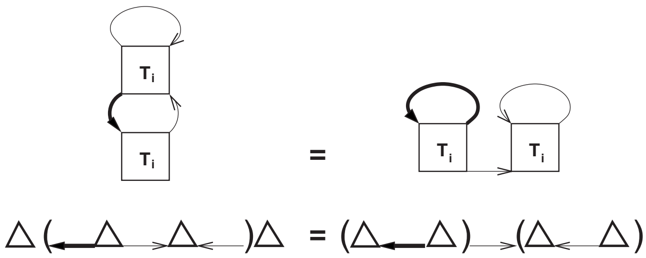

FIG. 1. Proof of relation (16) for singular channel T matrices which become separable. Thin lines denote the subtracted propagator (1) and thick lines the full propagator.

tion $\Sigma' = \Sigma_{j\neq i}\overline{T_j G}$ and for the singular channel $\Sigma_i = \overline{T_i G_{\bar i}}$. In the following, we will denote explicitly by which function the upper line is closed. All other products are understood as operator products of one-particle functions. For the above-mentioned averaged T-matrix approximation one has $K = G_{\bar i}$ and a closing by $\bar{G} \to c$ in terms of the impurity concentration c. In two-particle ladder approximation, one would have the form $K_i = G \cdot G_{\bar i}$. In the following we consider the general block K such that any more refined approximation can be chosen.

With Eq. (1) and $\Sigma_i = \overline{T_i \vec{G}_{\bar i}}$ we can write

$$1 = (1 - D)G^{-1}G_{\bar i} + DG^{-1}G_{\bar i} + G^{-1}G_{\bar i}\overline{T_i \vec{\bar{G}}_{\bar i}}G, \tag{12}$$

where we have added and subtracted an operator D which will be determined later by convenience. Now it is easy to proof with the help of the separability of the singular channel $T_i = \mp \Delta\Delta$ that the following relation holds:

$$\overline{T_i \vec{G}_{\bar i}}G = \overline{T_i \vec{\bar{G}}}G_{\bar i}. \tag{13}$$

Indeed we have with the help of Eq. (1),

$$\overline{T_i \vec{\bar{G}}}G_{\bar i}G^{-1} = \overline{T_i \vec{\bar{G}}} - \overline{T_i \vec{\bar{G}}}G_{\bar i}\overline{T_i \vec{G}_{\bar i}} \tag{14}$$

and

$$\overline{T_i \vec{G}_{\bar i}} = \overline{T_i \vec{G}} - \overline{T_i \overline{G_{\bar i}\Sigma_i} \vec{G}}. \tag{15}$$

Since we have the identity

$$\overline{T_i \overline{G_{\bar i}\Sigma_i}\vec{G}} = \overline{T_i \vec{\bar{G}}}G_{\bar i}\overline{T_i \vec{G}_{\bar i}} \tag{16}$$

as shown in Fig. 1, the Eqs. (14) and (15) are identical and relation (13) is proved.

Therefore we can write for Eq. (12)

$$1 = (1 - D)G^{-1}G_{\bar i} + (DG^{-1} + G^{-1}G_{\bar i}\overline{T_i \vec{\bar{G}}})G_{\bar i}. \tag{17}$$

Multiplying Eq. (1) from the right with $\overline{T_i \vec{G}_{\bar i}}$, we can find

$$G^{-1}G_{\bar i}\overline{T_i \vec{\bar{G}}} + \Sigma_i G_{\bar i}\overline{T_i \vec{\bar{G}}} = \overline{T_i \vec{\bar{G}}} = \overline{V\vec{\bar{G}}} + \overline{VKT_i \vec{\bar{G}}}, \tag{18}$$

where we have used Eq. (11) for the second identity. For the last term, we define now an effective potential $\tilde{V}_i$,

$$\tilde{V}_i G_{\bar i}\overline{T_i \vec{\bar{G}}} \equiv \overline{VKT_i \vec{\bar{G}}} \tag{19}$$

with the help of which we can invert Eq. (18),

$$G_{\bar i}\overline{T_i \vec{\bar{G}}} = (G^{-1} + \Sigma_i - \tilde{V}_i)^{-1}\overline{V\vec{\bar{G}}}. \tag{20}$$

Using this in Eq. (17), we arrive at

$$1 = (1 - D)G^{-1}G_{\bar i} + [1 + (\Sigma_i - \tilde{V}_i)G]^{-1}[(1 + \Sigma_i G)D - \tilde{V}_i GD + \overline{V\vec{\bar{G}}}G]G^{-1}G_{\bar i}. \tag{21}$$

Now we choose the operator D such that the last two terms cancel each other, i.e.,

$$\overline{V\vec{\bar{G}}}G \equiv \tilde{V}_i GD. \tag{22}$$

Using Eq. (1) in the form $G^{-1}G_{\bar i} = (1 + \Sigma_i G)^{-1}$ and subtracting from Eq. (21) the structure $1 = (1 - D)A^{-1}A + B^{-1}BD$ we obtain finally

$$\begin{aligned}(1 - D)(1 + \Sigma_i G)^{-1}\Sigma_i &= [1 + (\Sigma_i - \tilde{V})G]^{-1} \\ &\times[\tilde{V}_i GDG^{-1} - (1 + \Sigma_i G)D(1 + \Sigma_i G)^{-1}\Sigma_i]. \end{aligned}\tag{23}$$

Together with the operator [Eq. (22)] and the effective potential $\tilde{V}_i$ defined by Eq. (19) this is the desired generalized Soven equation. It is written in operator form which becomes an algebraic equation in the appropriate representation. In the operator form it is even valid in nonequilibrium and its time ordering can be treated, e.g., in the framework of generalized Kadanoff and Baym formalism[21] with the help the Langreth/Wilkins rules.[22]

Though introduced merely for mathematical convenience, the operator D corresponds to the concentration for impurity scattering and the effective potential corresponds to the effective potential in CPA. Therefore, D is called concentration operator hereafter.

Let us illustrate this with the help of special cases. Choosing the averaged T-matrix approximation we have only one-particle functions, $K = G_{\bar i}$ and the closing by the concentration as a c-number $\bar{G} \to c$, such that we get from Eq. (19) $\tilde{V}_i = V$ which gives with Eq. (22) $D = c$ such that the standard Soven equation[17] appears

$$(1 - c)\frac{\Sigma_i(p)}{1 + \Sigma_i(p)G(p)} = c\frac{V(p) - \Sigma_i(p)}{1 + [\Sigma_i(p) - V(p)]G(p)}. \tag{24}$$

As a second, so far not known, example we give the explicit expressions for the two-particle T matrix. Then $K = G \cdot G_{\bar i}$ is a product in spatial coordinates. Fourier transform of the difference coordinates and gradient expansion reveals then the structure $[p=(\mathbf{p},\omega_p)]$,

$$[1-D(p)]\frac{\Sigma_i(p)}{1+\Sigma_i(p)G(p)} = D(p)\frac{\tilde{V}_i(p)-\Sigma_i(p)}{1+[\Sigma_i(p)-\tilde{V}_i(p)]G(p)}. \tag{25}$$

The concentration operator takes the form

$$D(p) = \frac{\sum_{\bar{\mathbf{p}},\bar{\omega}} V(\bar{\mathbf{p}}-\mathbf{p}/2)G(-\bar{p})}{\tilde{V}_i(p)} = \frac{\Sigma_H(\mathbf{p})}{\tilde{V}_i(p)} \tag{26}$$

noting the Hartree self-energy Σ_H and the effective potential reads

$$\tilde{V}_i(p) = \frac{\overline{VKT_i\bar{G}}}{\overline{T_i\bar{G}}G_{\not i}} = \frac{\overline{T_i\bar{G}}G_{\not i} - \overline{V\bar{G}}}{\overline{T_i\bar{G}}G_{\not i}} = \frac{1}{G_{\not i}(p)} - \frac{\Sigma_H(\mathbf{p})}{\Sigma_i(p)G(p)}. \tag{27}$$

Here we have used Eq. (11) for the first equality and Eq. (13) for the second one. The channel T matrix reads explicitly

$$\Sigma_i(p) = \sum_{\bar{p}} T_i\left(\frac{\bar{\mathbf{p}}-\mathbf{p}}{2},\frac{\bar{\mathbf{p}}-\mathbf{p}}{2},p+\bar{\mathbf{p}},\omega_p+\omega_{\bar{p}}\right)G_{\not i}(-\bar{p}). \tag{28}$$

It is instructive to see that introducing Eqs. (26) and (27) into Eq. (25) leads indeed to an identity. This is due to the fact that we have assumed that all quantities such as T matrix and self-energy are known exactly. In case that we start with an approximation for the Green's function or self-energy we can use the above equation system and the generalized Soven form to iterate and to obtain approximations for the channel corrected propagators and self-energies.

To summarize it was shown that the Dyson equation can be rewritten exactly into a form containing anomalous propagators and self-energies if the repeated collisions in one channel are subtracted. The correction of the channel results into a self-energy which obeys a generalized Soven equation irrespective of the actually form of approximation used for the T matrix. This derived identity allows to improve any chosen approximation in the same way as the CPA does it with the averaged T-matrix approximation. The suggested procedure is to choose an approximation for the T matrix and to calculate the self-consistent channel-corrected propagators by iteration of Eqs. (26) and (27) and Eq. (25). Due to the versatile appearance of pairing and condensation phenomena ranging from nuclear, to solid state up to plasma physics, the systematic improvement of any approximation used and the underlying equivalences of the different approaches might be helpful. The superiority of the corrected T matrix considered in this Brief Report consists of the fact that the situation above and below the critical temperature, or in other words, the physics in and outside the condensate can be described with the help of the same theoretical approach.[4] First applications have shown already a better description of multiple phases in interacting Bose gases.[7] Further applications of the proposed scheme are in progress.

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