Conserving Gapless Mean-Field Theory for Weakly Interacting Bose Gases

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This paper presents a conserving gapless mean-field theory for weakly interacting Bose gases. We first construct a mean-field Luttinger-Ward thermodynamic functional in terms of the condensate wave function $\Psi$ and the Nambu Green’s function $\hat{G}$ for the quasiparticle field. Imposing its stationarity with respect to $\Psi$ and $\hat{G}$ yields a set of equations to determine the equilibrium for general non-uniform systems. They have a plausible property of satisfying the Hugenholtz-Pines theorem to provide a gapless excitation spectrum. Also, the corresponding dynamical equations of motion obey various conservation laws. Thus, the present mean-field theory shares two important properties with the exact theory: “conserving” and “gapless.” The theory is then applied to a homogeneous weakly interacting Bose gas with s-wave scattering length $a$ and particle mass $m$ to clarify its basic thermodynamic properties under two complementary conditions of constant density $n$ and constant pressure $p$. The superfluid transition is predicted to be first-order because of the non-analytic nature of the order-parameter expansion near $T_c$ inherent in Bose systems, i.e., the Landau-Ginzburg expansion is not possible here. The transition temperature $T_c$ shows quite a different interaction dependence between the $n$-fixed and $p$-fixed cases. In the former case $T_c$ increases from the ideal gas value $T_{0s}$ as $T_c/T_0 = 1 + 3.3a^2 / 2$, whereas it decreases in the latter as $T_c/T_0 = 1 - 3.84a(mp/2\pi^2)^{1/3}$. Temperature dependences of basic thermodynamic quantities are clarified explicitly.

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I. INTRODUCTION

Mean-field theories with self-consistency equations have played a central role in the development of our microscopic understanding on quantum many-particle systems, especially on broken-symmetry phases. One of the most outstanding examples is undoubtedly the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity, which may be regarded now as the Hartree-Fock theory in the Nambu space. In some notable cases like the BCS theory, mean-field theories have brought remarkable quantitative descriptions of experiments. At least, each mean-field theory has provided a basic starting point for later developments, as the Weiss and the Stoner theories for localized and itinerant ferromagnets, respectively. Hence there is every need for a mean-field theory of every quantum system. However, there has been no established mean-field theory for Bose-Einstein condensates (BEC).

Over the last sixty years, the field theory has manifested itself as one of the most powerful microscopic approaches to quantum many-particle systems. It was first applied to Bose particles in the celebrated work of Bogoliubov followed by intensive theoretical investigations in later years. However, it has brought a rather poor description of condensed Bose particles at finite temperatures. For example, we still do not have a complete agreement on the Bose-Einstein condensation temperature $T_c$ of the homogeneous weakly interacting Bose gas under constant density $n$, not to mention its thermodynamic properties over $0 \leq T \leq T_c$; see Refs. 12 and 13 for a review on the $T_c$ calculations. This situation is partly due to the absence of a well-established renormalized perturbation theory for Bose systems corresponding to the Luttinger-Ward theory on Fermi liquids. Indeed, important formal results on Bose systems have often been obtained with the bare perturbation theory, as in the case of the Hugenholtz-Pines theorem. However, the bare perturbation expansion itself is not very suitable for practical calculations due to the infrared divergences inherent in Bose systems. On the other hand, we still do not have a systematic approximation scheme of how to renormalize the condensate wave function and the quasiparticle Green’s function self-consistently without losing the physical essentials of condensed Bose particles.

The self-consistent Wick decomposition procedure has proved to be quite powerful for most quantum many-particle systems at finite temperatures and might be used also for Bose particles. The corresponding mean-field theory for condensed Bose systems is known now as the Girardeau-Arnovitt theory or the Hartree-Fock-Bogoliubov (HFB) theory. However, it predicts an energy gap in the excitation spectrum, in contradiction to the Hugenholtz-Pines theorem of declaring a gapless excitation. Thus, it has become customary to introduce a further approximation to the HFB theory, now generally called the “Popov” approximation of completely disregarding the anomalous quasiparticle pair correlation to recover a gapless excitation. When it is adopted to describe dynamics, however, the same approximation does not satisfy various conservation laws as required. Also, it is not clear whether it is permissible or not to neglect the pair correlation completely. Recently, Proukakis et al. have presented an improved gapless theory with finite pair correlation. However, it still does not satisfy the conservation laws. Thus, there has been no mean-field theory for condensed Bose systems that simultan-
ously carries the important properties of the exact theory pointed out by Hohenberg and Martin: “conserving” and “gapless.”

On the basis of these observations, we have recently formulated a new mean-field theory for BEC with the desired conserving gapless character. We here present a detailed description of the theory with several new results. As first shown by Baym for normal Fermi liquids and pointed out by Hohenberg and Martin for condensed Bose systems, various conservation laws are automatically satisfied in the “Φ derivative approximations” where the irreducible self-energy Σ is obtained as a derivative of some functional Φ = Φ(Γ) with respect to the renormalized Green’s function Γ. This relationship between Σ and Γ holds exactly for Fermi systems in equilibrium, as shown by Luttinger and Ward. Indeed, Φ was first introduced by Luttinger and Ward as part of the exact thermodynamic functional Ω = Ω[Γ]. It was later taken up by Baym to present a criterion for obtaining approximate dynamical equations with conservation laws. It thus follows that dynamical equations obtained from a Luttinger-Ward functional naturally obey the conservation laws. We hence ask the heuristic question here: Can we construct a mean-field Luttinger-Ward thermodynamic functional for BEC that also satisfies the Hugenholtz-Pines theorem? This is indeed possible as will be shown below. The predictions of the resulting mean-field theory on the homogeneous weakly interacting Bose gas will be presented later with an expression for ΔTc: this application hopefully will provide a deeper insight into the superfluidity and phase transition of still mysterious 4He. It should be noted that the same idea has been adopted more recently by Ivanov, Riek, and Knoll (IRK) in a different context of the O(N) model to present an apparently different thermodynamic functional. It will be shown, however, that their functional yields exactly the same equilibrium thermodynamic properties on weakly interacting Bose gases as the present one.

We finally provide three comments on terminology to remove possible confusions in advance. First, Gardines and Castin and Dum have presented an alternative description of BEC, which was called by Gardines as “particle-number conserving Bogoliubov method.” However, his terminology is completely different from the present “conserving” and we call their formulations as “number-fixed” descriptions of BEC. Indeed, his terminology is connected more closely with the equilibrium thermodynamics to denote the fact that the particle number N is chosen as an independent variable instead of the chemical potential µ. The two descriptions of using N and µ are equivalent in the thermodynamic limit except the fluctuation in the particle number. It is worth pointing out that a “number-fixed” theory does not necessarily provide “conserving” dynamical equations in the present sense. Second, the term “gapless” is relevant here to the single-particle excitation. Indeed, the collective excitation has another story and is gapless even in the Girardeau-Arnouwitt theory, as already shown by Takano. Third, it has been pointed out by Yukalov that the word “Popov” may not be suitable for the approximation of setting the anomalous pair amplitude equal to zero in the HFB theory. Indeed, this approximation was introduced by Sholmo already in 1964 and used later by Reatto and Straley. We can also find the same approximation later in the work of Baym and Grimmer on the σ model. We will call it as the “Sholmo” approximation instead of “Popov” following Reatto and Straley.

This paper is organized as follows. Section II presents a mean-field free-energy functional for general non-uniform systems and derives a closed set of equations to determine the thermodynamic equilibrium. Section III applies the formulation to the homogeneous weakly interacting Bose gas under constant density to clarify its basic thermodynamic properties. Section IV treats the same system under the complementary condition of constant pressure. Section V concludes the paper. Appendix A summarizes Feynman rules for the perturbation expansion with respect to the Nambu Green’s function. Appendix B provides a proof on the condensed Bose systems that the conservation laws are obeyed in the Φ derivative approximations. In Appendix C, the connection between the present and the IRK theories is clarified. Appendix D discusses the origin of a non-Hermitian eigenvalue problem in condensed Bose systems. Appendix E derives compact expressions for the equilibrium thermodynamic functional and the entropy. We put k_B = 1 throughout.

II. MEAN-FIELD EQUATIONS

A. Free-energy functional

We express the field operator ψ(r) as a sum of the condensate wave function Ψ(r) and the quasiparticle field φ(r) as

\[ \psi(r) = \Psi(r) + \phi(r). \]  \hspace{1cm} (1)

It is convenient to introduce the spinors:

\[ \phi \equiv \begin{bmatrix} \phi \\ \phi^\dagger \end{bmatrix}, \quad \phi^\dagger \equiv \begin{bmatrix} \phi^\dagger \\ \phi \end{bmatrix}, \]  \hspace{1cm} (2a)

\[ \Psi \equiv \begin{bmatrix} \Psi \\ \Psi^* \end{bmatrix}, \quad \Psi^\dagger \equiv \begin{bmatrix} \Psi^* \\ \Psi \end{bmatrix}. \]  \hspace{1cm} (2b)

Using Eq. 2a, we define our Matsubara Green’s function in Nambu space as

\[ \hat{G}(r, r'; \tau) \equiv -\hat{T}_3 \langle T_\tau \phi(r, \tau) \phi^\dagger(r') \rangle \]

\[ = T \sum_{n=-\infty}^{\infty} \hat{G}(r, r'; z_n) e^{-z_n \tau}, \]  \hspace{1cm} (3)
with \( \hat{\tau}_3 \) the third Pauli matrix and \( z_n \equiv 2\pi nT \). The factor \( \hat{\tau}_3 \) is usually absent in the definition of Green’s function.\textsuperscript{24,25} Introducing the factor brings an advantage that the eigenvalue problem for \( \hat{G}^{-1} \) is equivalent to the Bogoliubov-de Gennes (BdG) equation for the quasiparticles, as seen below. Thus, \( \hat{G} \) can be put into a diagonal form with respect to the eigenstates of the BdG equation.

The bare perturbation expansion for condensed Bose systems may also be performed quite compactly in terms of the Nambu-Matsubara Green’s function of Eq. (3). The corresponding Feynman rules can be found easily from those of the superconducting Fermi systems\textsuperscript{24} with slight modifications, which are summarized in Appendix A. Retaining the lowest-order diagrams in terms of the interaction and renormalizing \( \hat{G}_0 \rightarrow \hat{G} \), one may express the free-energy functional of the HFB theory in a Luttinger-Ward form\textsuperscript{34,55} with respect to \( \Psi \) and \( \hat{G} \).

We now present our mean-field Luttinger-Ward functional \( \Omega = \Omega(\Psi, \Psi^*, \hat{G}) \) which has been obtained from that of the HFB theory with a slight modification. It is given by

\[
\Omega = \int \Psi^*(\mathbf{r})K\Psi(\mathbf{r})\,d\mathbf{r} + \frac{T}{2} \sum_n \text{Tr} \left[ \ln(\hat{\tau}_3 K + \hat{\Sigma} - z_n \mathbf{1}) \right] + \hat{\Sigma} \mathbf{1}(z_n) + \Phi .
\]

Here \( K \) is defined by

\[
K = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) - \mu_n ,
\]

with \( V(\mathbf{r}) \) the external potential and \( \mu_n \) the chemical potential, \( \mathbf{1} \) is the unit matrix, and \( \mathbf{1}(z_n) \) denotes

\[
\mathbf{1}(z_n) = \begin{bmatrix}
e^{z_n 0_+} & 0 \\
0 & e^{-z_n 0_+}
\end{bmatrix} ,
\]

with \( 0_+ \) an infinitesimal positive constant. The branch cut of the logarithm in Eq. (4) is chosen along the negative real axis, and \( \text{Tr} \) here includes an integration over space variables with multiplications of \( \hat{\tau}_3 K \) and \( -z_n \mathbf{1} \) by \( \delta(\mathbf{r} - \mathbf{r}') \) from the right implied. Finally, \( \hat{\Sigma} \) denotes the irreducible self-energy obtained from the functional \( \Phi = \Phi(\Psi, \Psi^*, \hat{G}) \) by

\[
\hat{\Sigma}(\mathbf{r}, \mathbf{r}'; z_n) = -\frac{2}{T} \frac{\delta \Phi}{\delta \hat{G}(\mathbf{r}', \mathbf{r}; z_n) .}
\]

With Eq. (10), \( \Omega \) becomes stationary with respect to a variation in \( \hat{G} \) satisfying Dyson’s equation:

\[
\hat{G}^{-1} = z_n \mathbf{1} - \hat{\tau}_3 K - \hat{\Sigma} .
\]

The condensate wave function \( \Psi(\mathbf{r}) \) in equilibrium is also determined by \( \delta \Omega / \delta \Psi^*(\mathbf{r}) = 0 \). Noting \( \delta \Omega / \delta \hat{G} = 0 \), we only need to consider the explicit \( \Psi^* \) dependences in \( \Omega \) to obtain

\[
K\Psi(\mathbf{r}) = -\eta(\mathbf{r}) ,
\]

with

\[
\eta(\mathbf{r}) = \frac{\delta \Phi}{\delta \Psi^*(\mathbf{r})} .
\]

The quantity \( \eta(\mathbf{r}) \) is the so-called condensate source function.\textsuperscript{24,25} Equations (7) and (10) constitute the \( \Phi \)-derivative approximation\textsuperscript{24} where the conservation laws are obeyed automatically by the dynamical equations. This is one of the main advantages in using the Luttinger-Ward functional as a starting point.

Despite their importance, the conservation laws in the \( \Phi \)-derivative approximation seems not to have been described to an enough extent in the literature for the condensed Bose systems. We hence provide a detailed proof of them in Appendix B.

A key quantity in Eq. (10) is \( \Phi \). We choose it so that the Hugenholtz-Pines theorem is satisfied simultaneously. Explicitly, it is given by

\[
\Phi = \int d\mathbf{r} \int d\mathbf{r}' \mathcal{U}(\mathbf{r} - \mathbf{r}') \left[ \frac{1}{2} |\Psi(\mathbf{r})|^2 |\Psi(\mathbf{r}')|^2 
\right.

\[
- \frac{T}{2} \sum_n |\Psi(\mathbf{r})|^2 \text{Tr} \hat{\tau}_3 \hat{G}(\mathbf{r}', \mathbf{r}; z_n) \mathbf{1}(z_n)
\]

\[
- \frac{T}{2} \sum_n \text{Tr} \hat{\tau}_3 \hat{\Psi}(\mathbf{r}') \hat{\Psi}^\dagger(\mathbf{r}') \hat{G}(\mathbf{r}', \mathbf{r}; z_n) \mathbf{1}(z_n)
\]

\[
+ \frac{T^2}{8} \sum_{n,n'} \text{Tr} \hat{\tau}_3 \hat{G}(\mathbf{r}, \mathbf{r}; z_n) \mathbf{1}(z_n) \text{Tr} \hat{\tau}_3 \hat{G}(\mathbf{r}', \mathbf{r}'; z_{n'}) \mathbf{1}(z_{n'})
\]

\[
+ \frac{T^2}{8} \sum_{n,n'} \text{Tr} \hat{G}(\mathbf{r}, \mathbf{r}'; z_n) \mathbf{1}(z_n) \hat{G}(\mathbf{r}', \mathbf{r}; z_{n'}) \mathbf{1}(z_{n'}) \right] ,
\]

where \( \mathcal{U} \) denotes the interaction potential. As may be realized from Appendix A where the Feynman rules in Nambu space are given explicitly, the five terms in the square brackets of Eq. (11a) corresponds to the diagrams of Fig. 1(a)-(e), respectively. The difference of Eq. (11a) from \( \Phi_{\text{HFB}} \) lies in the Fock terms, i.e., the third and the fifth terms. Indeed, \( \Phi_{\text{HFB}} \) is recovered from Eq. (11a) by replacing \( \hat{G} \) and \( \hat{\tau}_3 \hat{\Psi}(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}') \) in the two Fock terms by \( \hat{\tau}_3 \hat{G} \) and \( \hat{\Psi}(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}') \), respectively; the present functional was found in the reverse way.

At this stage, it may be worth providing a comment on the present functional. As mentioned by Shi and Griffiths\textsuperscript{22,24} the HFB approximation yields over-counting of the off-diagonal self-energy diagrams in the bare perturbation expansion, thereby leading to an unphysical energy gap in the excitation spectrum. Hence it is necessary to subtract the extra contributions from the HFB self-energy. In this context, it is interesting to note that the present functional removes some of the off-diagonal terms in \( \Phi_{\text{HFB}} \) as

\[
\Phi = \Phi_{\text{HFB}} - \int d\mathbf{r} \int d\mathbf{r}' \mathcal{U}(\mathbf{r} - \mathbf{r}') \left[ \Psi(\mathbf{r}) \Psi^\dagger(\mathbf{r}') \phi(\mathbf{r}') \phi(\mathbf{r}) 
\right.

\[
+ \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r}') \phi(\mathbf{r}) \phi^\dagger(\mathbf{r}') + |\phi(\mathbf{r}) \phi(\mathbf{r}')|^2 \right] .
\]
It satisfies the Hugenholtz-Pines relation appropriately to be free from the unphysical excitation gap, as seen below. Thus, the subtraction mentioned above may have been performed appropriately.

Based on exactly the same idea as adopted here, Ivanov, Riek, and Knoll have recently constructed an alternative functional $\Phi_{IRK}$ for the $O(N)$ model so as to satisfy the Hugenholtz-Pines theorem. Their functional is given in the present context by

$$\Phi_{IRK} = \Phi_{HFB} - \int \mathrm{d}r \int \mathrm{d}r' U(r-r')|\langle \phi(r)\phi(r') \rangle|^2.$$  \hfill (12)

In spite of the apparent difference between Eqs. (11b) and (12), however, $\Phi$ and $\Phi_{IRK}$ lead to exactly the same thermodynamic properties for weakly interacting Bose gases, as shown in Appendix C.

**B. Equilibrium solution**

Now that $\Phi$ is given explicitly, we obtain the equilibrium self-energy by Eq. (7). It may be written as

$$\hat{\Sigma}(r,r') = \left[ \begin{array}{cc} \Sigma(r,r') & \Delta(r,r') \\ -\Delta^*(r,r') & -\Sigma^*(r,r') \end{array} \right],$$  \hfill (13)

where $\Sigma$ and $\Delta$ are given by

$$\Sigma(r,r') = \delta(r-r') \int U(r-r'') \rho(r'',r) \mathrm{d}r'',$nolines
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$$+ U(r-r') \rho(r,r'),$$  \hfill (14a)

$$\Delta(r,r') = U(r-r') \rho(r,r'),$$  \hfill (14b)

respectively, with

$$\rho(r,r') = \Psi(r)\Psi^*(r') + \langle \phi(r')\phi(r) \rangle,$$  \hfill (15a)

$$\tilde{\rho}(r,r') = \Psi(r)\Psi(r') + \langle \phi(r)\phi(r') \rangle.$$  \hfill (15b)

The equation for the condensate wave function in equilibrium is obtained from Eqs. (10), (11), and (14). It can be written explicitly in terms of Eq. (13) by

$$K \Psi(r) + \int [\Sigma(r,r')\Psi(r') - \Delta(r,r')\Psi^*(r')] \mathrm{d}r' = 0.$$  \hfill (16)

In the homogeneous case with no external potential where $K \to -\mu_s$ and $\Psi = \sqrt{n_0}$ with $n_0$ the condensate density, Eq. (16) reduces to the Hugenholtz-Pines relation $\mu_s = E_{k=0}^* - \Delta_{k=0}$, as desired. The expression for the particle number $N = -\partial \Omega/\partial \mu_s$ is found similarly as

$$N = \int \rho(r,r) \mathrm{d}r,$$  \hfill (17)

with $\rho$ given by Eq. (15b). Using this equation, one may change independent variables of the free energy as $\Omega(T,V,\mu) \to F(T,V,N) = \Omega(T,V,\mu) + \mu N$. Equations (8) and (13)-17 determine the equilibrium.

**C. Bogoliubov-de Gennes equations**

Physical quantities in equilibrium may be calculated most conveniently in the representation where $\hat{G}$ is diagonal. Noting Eq. (13), we introduce

$$\tilde{\hat{H}}(r,r') = \hat{\Sigma}(r-r') + \hat{\Delta}(r,r').$$  \hfill (18)

The eigenvalue problem for $\hat{\tilde{H}}$ constitutes the BdG equation:

$$\int \tilde{H}(r,r') \varphi_\mu^\dagger(r') \mathrm{d}r' = E_\mu \varphi_\mu(r),$$  \hfill (19a)

where $\varphi_\mu$ denotes an eigenfunction. It has a peculiar feature that $\tilde{H}$ is not Hermitian but satisfies $\tilde{H}^\dagger(r,r') = \tilde{\tau}_3 \tilde{H}(r',r) \tilde{\tau}_3$. Since most of the eigenvalue problems in quantum mechanics are Hermitian by nature, it may be worth tracing why we have to treat a non-Hermitian matrix in BEC. It is shown in Appendix D that this symmetry necessarily results from the requirement that the quasiparticle field obey the Bose statistics.

Let us enumerate basic properties of the BdG equation, since this seems not to have been performed to an enough extent in the literature. We will also provide a compact Nambu representation to every quantity of the BdG equation. Taking its Hermitian conjugate and using $\tilde{H}^\dagger(r,r') = \tilde{\tau}_3 \tilde{H}(r',r) \tilde{\tau}_3$, Eq. (19a) may be written alternatively as

$$\int \varphi_\mu^\dagger(r) \tilde{\tau}_3 \tilde{H}(r,r') \tilde{\tau}_3 \mathrm{d}r = E_\mu \varphi_\mu^\dagger(r).$$  \hfill (19b)

Let us multiply Eq. (19a) by $\varphi_\mu^\dagger(r) \tilde{\tau}_3$ from the left and integrate it over $r$. Similarly, we multiply Eq. (19a) by $\varphi_\mu(r')$ from the right and integrate it over $r'$. Subtracting the latter from the former, we obtain

$$E_\mu - E_\mu^* = (\varphi_\mu^\dagger \varphi_\mu) |\tilde{\tau}_3 \tilde{\tau}_3^\dagger \varphi_\mu = 0.$$  \hfill (20)
We first put $\mu' = \mu$ in Eq. (20). We then realize that $E_\mu$ is real as long as $\langle \tilde{\varphi}_\mu | \tilde{\varphi}_\mu \rangle \neq 0$ can be satisfied by the eigenstate. We assume that (i) this is the case and (ii) eigenstates with positive eigenvalues may be normalized as $(\langle \tilde{\varphi}_\mu | \tilde{\varphi}_\mu \rangle)^{1/2} = 1$. We next consider the case $E_\mu' \neq E_\mu$ in Eq. (21). We then find that the two eigenstates with different eigenvalues are orthogonal as $(\langle \tilde{\varphi}_\mu' | \tilde{\varphi}_\mu \rangle) = 0$.

The Hamiltonian $\hat{H}$ has another symmetry: $\hat{H}(r, r') = -\tau_f \hat{H}(r, r') \tau_f$ with $\tau_f$ the first Pauli matrix. Let us take the complex conjugate of Eq. (13a), multiply it by $-\tau_f$ from the left, and use the above symmetry. It is thereby shown that a positive eigenvalue $E_\nu$ of the BdG equation with the eigenfunction:

$$
\tilde{u}_\nu(r) \equiv \begin{bmatrix} u_\nu(r) \\ -v_\nu(r) \end{bmatrix},
$$

is always accompanied by the negative eigenvalue $-E_\nu$ with the eigenfunction:

$$
\tilde{v}_\nu(r) \equiv \begin{bmatrix} -v_\nu(r) \\ u_\nu(r) \end{bmatrix}.
$$

The sign in front of $v_\nu^*$ is introduced for convenience to make the coefficient $v_\nu$ of the homogeneous system positive. As mentioned above, we assume that $\tilde{u}_\nu(r)$ with $E_\nu > 0$ can be normalized as

$$
\langle u_\nu | u_\nu \rangle - \langle v_\nu | v_\nu \rangle = 1.
$$

Violation of this condition marks an instability of the assumed $\Psi(r)$, as is the case of a vortex-free $\Psi(r)$ under an angular velocity $\Omega$ beyond the critical value $\Omega_c$.

It also follows from Eq. (14) that the BdG equation has eigenvalue 0 whose eigenfunction is proportional to $\tilde{\varphi}_0$ with $\tilde{\varphi}_\nu$ given by Eq. (20). We adopt the following normalized eigenfunction for this state:

$$
\tilde{\varphi}_0^{(1)}(r) \equiv \frac{1}{\langle \tilde{\varphi}_\nu | \tilde{\varphi}_\nu \rangle^{1/2}} \tilde{\varphi}_\nu = \begin{bmatrix} \varphi_0(r) \\ -\varphi_0^*(r) \end{bmatrix}.
$$

It is orthogonal to $\tilde{u}_\nu$ as $\langle \tilde{u}_\nu | \tilde{\varphi}_0^{(1)} \rangle = 0$, i.e., $\langle u_\nu | \varphi_0 \rangle = \langle \varphi_0 | v_\nu \rangle$. Noting Eq. (21c), we may assume

$$
\langle u_\nu | \varphi_0 \rangle = \langle v_\nu | \varphi_0 \rangle = 0.
$$

There still remains another independent state:

$$
\varphi_0^{(2)}(r) \equiv \tilde{\varphi}_0^{(1)}(r) = \begin{bmatrix} \varphi_0(r) \\ \varphi_0^*(r) \end{bmatrix},
$$

which does not belong to $\hat{H}$, however. The functions $\varphi_0^{(j)}(r) (j = 1, 2)$ satisfy $\langle \varphi_0^{(j)} | \tilde{\varphi}_0 \rangle = 1 - \delta_{ij}$.

The functions $|\tilde{u}_\nu\rangle$, $|\tilde{v}_\nu\rangle$, $|\varphi_0^{(1)}\rangle$, and $|\varphi_0^{(2)}\rangle$ are assumed to form a complete set. As shown by expanding an arbitrary spinor with respect to the basis functions and calculating the corresponding expansion coefficients, this statement is equivalent to

$$
\sum_\nu (|\tilde{u}_\nu\rangle \langle \tilde{u}_\nu | \tilde{\varphi}_0 \rangle - |\tilde{v}_\nu\rangle \langle \tilde{v}_\nu | \tilde{\varphi}_0 \rangle) + |\varphi_0^{(1)}\rangle \langle \varphi_0^{(1)} | \tilde{\varphi}_0 \rangle + |\varphi_0^{(2)}\rangle \langle \varphi_0^{(2)} | \tilde{\varphi}_0 \rangle = \hat{1}.
$$

In summary, the BdG equation for a pair of eigenstates $\pm E_\nu$ ($E_\nu > 0$) can be written compactly in a matrix form as

$$
\int \hat{H}(r, r') \tilde{u}_\nu(r') \, dr' = \tilde{u}_\nu(r) E_\nu \tilde{\varphi}_3,
$$

where $\tilde{u}_\nu$ is defined by

$$
\tilde{u}_\nu(r) = \begin{bmatrix} u_\nu(r) & -v_\nu(r) \end{bmatrix}.
$$

There exists another independent state composed of the condensate wave function $\Psi(r)$:

$$
\varphi_0(r) = \begin{bmatrix} \varphi_0(r) \\ -\varphi_0^*(r) \end{bmatrix},
$$

with $N_0 \equiv \frac{1}{2} \langle \tilde{\Psi} | \tilde{\Psi} \rangle$ denoting the condensate number. The orthonormality of the basis functions reads

$$
\int \tilde{\varphi}_0^{(1)}(r) \tilde{\varphi}_3 \varphi_0(r) \, dr = \delta_{\nu, 0} \hat{1},
$$

$$
\int \tilde{\varphi}_0^{(1)}(r) \tilde{\varphi}_3 \varphi_0(r) \, dr = \hat{1},
$$

$$
\int \tilde{\varphi}_0^{(2)}(r) \tilde{\varphi}_3 \varphi_0(r) \, dr = 0.
$$

The completeness can be written alternatively as

$$
\sum_\nu \tilde{u}_\nu(r) \tilde{\varphi}_3 \tilde{u}_\nu(r') = \tilde{\varphi}_0(r) \tilde{\varphi}_0(r') + \varphi_0(r) \varphi_0(r') = 0,
$$

as seen by writing down the matrix elements explicitly. Equations (24) - (27) are the basic properties of the eigenstates of the BdG equation. Noting that $\varphi_0^{(2)}(r)$ is absent in $\hat{H}$, Eq. (15) may be expanded as

$$
\hat{G}(r, r' ; z) = \sum_\nu \tilde{u}_\nu(r) \tilde{\varphi}_3 \tilde{u}_\nu(r') \tilde{\varphi}_3 \tau_3,
$$

Green’s function $\hat{G} = (z_n \hat{1} - \hat{H})^{-1}$ becomes diagonal in the representation where $\hat{H}$ is. In addition, eigenvalue 0 is absent in $\hat{G}$. Hence $\hat{G}(r, r' ; z_n)$ can be written as

$$
\hat{G}(r, r' ; z_n) = \sum_\nu \tilde{u}_\nu(r) \tilde{\varphi}_3 \tilde{u}_\nu(r') \tilde{\varphi}_3 \tau_3,
$$

with

$$
\hat{G}_\nu(z_n) = \begin{bmatrix} (z_n - E_\nu)^{-1} & 0 \\ 0 & (z_n + E_\nu)^{-1} \end{bmatrix}.
$$

Substituting Eq. (29) into Eq. (29) and performing summation over $z_n$ with $\tau = -0_+$, we obtain the expressions for $(\phi^{(1)}(r') \phi(r))$ and $(\phi(r) \phi(r'))$ as

$$
(\phi^{(1)}(r') \phi(r)) = \sum_\nu [u_\nu(r) u_\nu^*(r') n_\nu + v_\nu(r) v_\nu^*(r')(1 + n_\nu)],
$$

(30a)
\[ (\phi(r)\phi(r')) = \frac{1}{2} \sum \nu [u_\nu(r)v_\nu(r') + v_\nu(r)u_\nu(r')] (1 + 2n_\nu), \]

(30b)

where \( n_\nu \equiv (e^{E_\nu/T} - 1)^{-1} \) is the Bose distribution function, and we have used the (1, 2) element of Eq. (27) to make Eq. (30b) manifestly symmetric with respect to \( r \) and \( r' \).

Equations (16), (24), and (30) form a closed set of self-consistent equations satisfying both the Hugenholtz-Pines theorem and various conservation laws. Note that the pair correlation \( \langle \phi\phi \rangle \) is adequately included in Eqs. (16), (24), and (30b); neglecting this contribution yields the Sholno theory.

D. Expressions of equilibrium

It is shown in Appendix E that we can transform Eq. (14) in equilibrium into

\[ \Omega_{eq} = T \sum \nu \ln(1 - e^{-E_\nu/T}) - \sum \nu E_\nu \int |v_\nu(r)|^2 dr \]

\[ - \frac{1}{2} \int dr \int dr' \left[ \Sigma(r, r') \rho(r', r) - \Delta(r, r') \hat{\rho}(r', r) \right]. \]

(31)

The entropy in equilibrium can be obtained from \( S_s = -\partial \Omega_{eq} / \partial T \) by differentiating Eq. (14) in terms of the explicit \( T \) dependences. As shown in Appendix E, this yields

\[ S_s = \sum \nu [(1 + n_\nu) \ln(1 + n_\nu) - n_\nu \ln n_\nu]. \]

(32)

This completes the formulation of our mean-field theory.

III. HOMOGENEOUS GAS UNDER CONSTANT DENSITY

A. Equations of equilibrium

We now apply the previous formalism to a homogeneous weakly interacting Bose gas with volume \( V \) and particle number \( N \). The interaction we adopt is given by

\[ U(r - r') = \frac{4\pi \hbar^2 a}{m} \delta(r - r'), \]

(33)

where \( m \) is the particle mass and \( a \) is the s-wave scattering length. The important dimensionless parameter of the system is given by

\[ \delta = a n^{1/3}, \]

(34)

with \( n \equiv N/V \), which completely characterizes the properties of \( \delta \ll 1 \).

The corresponding condensate wave function and the quasiparticle eigenfunctions are the plane waves:

\[ \Psi(r) = \sqrt{n_0}, \]

(35)

\[ \hat{u}_k(r) = \frac{1}{\sqrt{V}} e^{ikr} \begin{bmatrix} u_k - v_k \\ -v_k - u_k \end{bmatrix}, \]

(36)

with \( n_0 \equiv N_0/V \) denoting the condensate density. It should be pointed out that the definition of \( \hat{u}_k(r) \) above is slightly different from Eq. (30b). Indeed, \( \hat{u}_k(r) \) is composed of \( \hat{u}_k(r) \) and \( -\hat{u}_k^*(r) \) with the common spatial dependence \( e^{ikr} \), which is more convenient for the homogeneous case. The coefficients \( u_k \) and \( v_k \) are chosen real; they clearly have the symmetry: \( u_{-k} = u_k \) and \( v_{-k} = v_k \).

Accordingly, Eq. (13) can be expanded as

\[ \hat{\Sigma}(r, r') = \frac{1}{V} \sum_k e^{ik(r-r')} \begin{bmatrix} \Sigma & \Delta \\ -\Delta & -\Sigma \end{bmatrix}, \]

(37)

where the coefficients \( \Sigma \) and \( \Delta \) have no \( k \) dependence for the contact interaction. The Hartree-Fock energy \( \Sigma \) is obtained from Eqs. (15a), (17), and (38) as

\[ \Sigma = \frac{8\pi \hbar^2 a}{m}. \]

(38)

It merely shifts the chemical potential and does not play an important role in the thermodynamics with constant density. Substitution of Eqs. (35) and (37) into Eq. (16) yields the Hugenholtz-Pines relation:

\[ \mu_s = \Sigma - \Delta. \]

(39)

Hence the excitation spectrum has no energy gap in our mean-field theory.

The quasiparticle eigenstates are obtained by substituting Eqs. (35) and (37) into Eqs. (13) and (24) and diagonalizing the resulting \( 2 \times 2 \) matrix in \( k \) space. We thereby arrive at the well-known expressions:

\[ E_k = \sqrt{\epsilon_k (\epsilon_k + 2\Delta)}, \]

(40a)

\[ u_k = \sqrt{\frac{\xi_k + E_k}{2E_k}}, \quad v_k = \sqrt{\frac{\xi_k - E_k}{2E_k}}, \]

(40b)

with \( \epsilon_k = \hbar^2 k^2/2m \) and \( \xi_k = \epsilon_k + \Delta \). Putting them back into Eqs. (14a) and (17), with Eq. (30), we obtain

\[ n = n_0 + A \left( \int_0^\infty \frac{\xi^{1/2}}{E} e^{E/T - 1} d\xi + \sqrt{\frac{\pi}{3}} \Delta^{3/2} \right), \]

(41)

\[ \Delta = \frac{4\pi \hbar^2 a}{m} \left[ n_0 + A \left( \int_0^\infty \frac{\Delta^{1/2}}{E} e^{E/T - 1} d\xi + \Delta^{1/2} \right) \right], \]

(42)
where \( A = m^{3/2}/\sqrt{2\pi^2 h^3} \) is a numerical constant, and we have introduced an energy cutoff \( \varepsilon_c \) in Eq. \( \text{(12)} \) to remove an ultraviolet divergence inherent in the contact interaction. Equations \( \text{(11)} \) and \( \text{(12)} \) forms coupled self-consistent equations for \( n_0 \) and \( \Delta \), which completely determines the thermodynamic equilibrium at a given temperature.

Once \( n_0 \) and \( \Delta \) are obtained by Eqs. \( \text{(11)} \) and \( \text{(12)} \), we can calculate equilibrium thermodynamic properties such as the pressure \( p_s \), the entropy \( S_s \), and the superfluid density \( \rho_s \). Pressure \( p_s = -\Omega_{eq}/V \) is transformed from Eq. \( \text{(11)} \) into

\[
p_s = \frac{\Sigma}{2} n_0 - \frac{\Delta}{2} n_0 + A \int_0^\infty \left( \frac{2\varepsilon \Delta^2}{3E} - \varepsilon^{1/2} \right) \frac{\varepsilon^{1/2}}{e^{E/T} - 1} \, d\varepsilon - \frac{A}{15\sqrt{2}} \Delta^{5/2}.
\]

Equation \( \text{(43)} \) for \( S_s \) now reads

\[
\frac{S_s}{N} = \frac{A}{nT} \int_0^\infty \frac{5\xi + 3\Delta}{3E} \frac{\varepsilon^{3/2}}{e^{E/T} - 1} \, d\varepsilon.
\]

The expression of \( \rho_s \) is given by \( \text{(30)} \)

\[
\rho_s = mn \left[ 1 - \frac{2A}{3nT} \int_0^\infty \frac{\varepsilon^{3/2} e^{E/T}}{(e^{E/T} - 1)^2} \, d\varepsilon \right].
\]

The constant \( A \) in Eqs. \( \text{(11)} \)–\( \text{(15)} \) under constant density may be written alternatively in terms of the transition temperature of the ideal Bose gas \( T_0 = (2\pi \hbar^2/m) \left[ n / \zeta(\frac{3}{2}) \right]^{2/3} \) as

\[
A = \frac{2n}{\sqrt{\pi \zeta(\frac{3}{2})} T_0^{3/2}},
\]

with \( \zeta(\frac{3}{2}) = 2.61 \) denoting the Riemann \( \zeta \) function. It is convenient to choose \( T_0 \) as the unit of energy. Then Eq. \( \text{(42)} \), for example, reads

\[
\left[ 1 - \frac{4\varepsilon_c^{1/2} \Delta}{\sqrt{\pi \zeta(\frac{3}{2})} T_0^{1/3} E} \right] + \frac{2}{\sqrt{\pi \zeta(\frac{3}{2})}} \int_0^\infty \frac{\Delta}{E} \frac{\varepsilon^{1/2}}{e^{E/T} - 1} \, d\varepsilon \right].
\]

We choose the cutoff \( \varepsilon_c \), so that \( 1 \ll \varepsilon_c \ll 3\Delta^{-2} \) is satisfied and neglect the cutoff-dependent term in the following. This does not affect the results qualitatively, and even quantitatively to the leading order in \( \Delta \).

Numerical calculations of Eqs. \( \text{(11)} \)–\( \text{(15)} \) can be performed easily to clarify temperature dependences of the basic thermodynamic quantities in the condensed phase. A change of variable \( \varepsilon = 2\Delta \sinh^2 t \) is found to improve convergence of the integrations including \( e^{E/T} \). The corresponding equations for the normal state are obtained from Eqs. \( \text{(11)} \), \( \text{(13)} \), and \( \text{(14)} \) by setting \( \Delta = n_0 = 0 \) and \( E = \xi = \varepsilon + \Sigma - \mu_n \), which yield \( \mu_n \), \( p_n \), and \( S_n \) as a function of \( T \). The transition temperature \( T_c \) is then determined by the thermodynamic condition \( F_n(T_c, V, N) = F_n(T_0, V, N) \) appropriate under constant volume. The specific heat \( C \) may be calculated from the results on \( S \) by numerical differentiations.

### B. Properties near \( T_c \)

We now investigate the properties near \( T_c \) \((\sim T_0 = 1)\) in more detail. To this end, we make use of the following asymptotic expansions for the integrals in Eqs. \( \text{(11)} \)–\( \text{(13)} \), respectively:

\[
\frac{2}{\sqrt{\pi \zeta(\frac{3}{2})}} \int_0^\infty \frac{\varepsilon^{1/2}}{e^{E/T} - 1} \, d\varepsilon = T^{3/2}(1 - b_1 x^{1/2})
\]

\[
\frac{2}{\sqrt{\pi \zeta(\frac{3}{2})}} \int_0^\infty \frac{\Delta}{E} \frac{\varepsilon^{1/2}}{e^{E/T} - 1} \, d\varepsilon = T^{3/2} b_1 x^{1/2}
\]

\[
\frac{2}{\sqrt{\pi \zeta(\frac{3}{2})}} \int_0^\infty \frac{(2\varepsilon \Delta^2 - \Delta^2)}{3E} \frac{\varepsilon^{1/2}}{e^{E/T} - 1} \, d\varepsilon = T^{5/2}(1 - b_1 y + b_2 y^{3/2})
\]

with \( x = \Delta/T \), \( b_1 = \sqrt{2\pi / \zeta(\frac{3}{2})} = 0.960 \), \( b_1' = \zeta(\frac{3}{2}) \zeta(\frac{5}{2}) = 1.95 \), and \( b_2 = 5/\sqrt{2\pi} / \zeta(\frac{7}{2}) = 1.56 \). Each expression of Eq. \( \text{(48a)} \) has been obtained as follows: (i) Expand the integrand in terms of \( \Delta \) up to the order where the integral converges to obtain the leading terms analytic in \( x \). (ii) Subtract the leading contribution from the original integral to express the residual term as an integral. (iii) Estimate the higher-order integral by expanding the exponentials in the denominators up to the first order. For example, analytic terms are absent in Eq. \( \text{(48a)} \), and the integral has been estimated by approximating \( e^{E/T} - 1 \approx E/T \) in the denominator. Those residual integrals generally yield terms non-analytic in \( x \). This non-analyticity in the expansion near \( T_c \) is inherent in Bose systems stemming from the divergence of the Bose distribution function at zero energy. This is in marked contrast to the weak-coupling theory of superconductivity where the gap equation near \( T_c \) is analytic in \( x^2 \equiv (\Delta/T)^2 \) to make the Landau-Ginzburg expansion possible. Thus, unlike the Ginzburg-Landau equations for superconductors, the Ginzburg-Pitaevskii equation for the condensed Bose systems cannot be justified microscopically. It is this non-analyticity which turns the mean-field transition into first order and also brings various anomalies in the thermodynamic properties near \( T_c \) which cannot be described by the Landau theory of second-order transition. Substituting Eqs. \( \text{(48a)} \) and \( \text{(48b)} \) into Eqs. \( \text{(11)} \) and \( \text{(12)} \), respectively, we obtain

\[
\frac{n_0}{n} = 1 - T^{3/2}(1 - b_1 y + b_2 y^{3/2})
\]
\[
\begin{align*}
\frac{n_0}{n} &= \frac{1 + b'_2 c T^{1/2} \delta}{c \delta} T y \left( y - \frac{b_1 c T^{1/2} \delta}{1 + b_2 c T^{1/2} \delta} \right), \\
\text{with } y &= x^{1/2} = (\Delta/T)^{1/2}, \quad b_2 = 0.559, \quad b'_2 = 1.12, \quad c = 2 \zeta(2)^{2/3} = 3.79. \quad \text{Here we have used the results of Eqs. (38a) and (38b), including higher-order terms } b_2 x \text{ and } -b'_2 x, \text{ respectively, with } b_2 \text{ and } b'_2 \text{ estimated numerically. Let us set Eq. (40) from Eq. (40a).}
\end{align*}
\]

Solving the resulting equation, we obtain \( y(T) \) as a function of \( T \) as
\[
y(T) = \frac{b_1 c T^{1/2} \delta}{1 + (b_2 + b'_2) c T^{1/2} \delta} \left\{ 1 + \left[ 1 - \frac{T - \frac{1}{2} - T^{-2}}{b_1 c \delta} \right] \right\}^{1/2}.
\]

The transition temperature \( T_c \) may be estimated by setting \( n_0 = 0 \) in Eq. (49), which yields
\[
y(T_c) = \frac{b_1 c T^{1/2} \delta}{1 + b_2 c T^{1/2} \delta} = 0.
\]

Equation (50) can be solved by expanding \( T_c \) in powers of \( \delta \) as
\[
T_c = 1 + \frac{8 \pi}{3 \zeta(2)^{1/3}} \delta + \frac{8 \pi}{3 \zeta(2)^{1/3}} \frac{14 \pi}{3 \zeta(2)^{1/3}} (b_2 + b'_2) c \delta^2
\]
\[
= 1 + 2.3 \delta^2 + \cdots.
\]

Thus, \( T_c \) initially increases linearly with \( \delta \). The numerical coefficient 2.33 agrees with the analytic result by Baym et al.\(^{33}\) as well as the numerical one by Holzmann and Krauth.\(^{33}\) It is worth pointing out that this expression makes the coefficients of \( \delta^0 \) and \( \delta \) in the large square bracket of Eq. (50) vanish at \( T_c \). Substituting Eq. (51) into Eq. (52) and noting \( y \equiv (\Delta/T)^{1/2} \), we obtain
\[
\Delta(T_c) = \frac{8 \pi}{3 \zeta(2)^{1/3}} \delta^2 = 13.3 \delta^2,
\]
to the leading order in \( \delta \). A comment is necessary on Eq. (52) at this stage. The expression (52) has been obtained as the highest temperature of the non-trivial solutions to Eq. (49). However, the corresponding superfluid transition is first-order. It hence follows that, under the present conditions of fixed \( V \) and \( N \), the transition temperature should have been determined alternatively by the requirement that the free energy \( F(T,V,N) \) be equal between the normal and superfluid phases. It will be shown below Eq. (52), however, that Eq. (52) indeed satisfies the requirement up to the order \( \delta^2 \).

We next consider the region below \( T_c \) and expand \( y(T) - y(T_c) \) in powers of \( 1 - T/T_c \). As noted below Eq. (52), the leading term at \( T_c \) in the large square bracket of Eq. (51) is proportional to \( \delta^2 \). The proportionality constant is found to be \( (b_2 c)^2 \) from the equation of order \( \delta^3 \) in the expansion of Eq. (52). Due to this smallness of the constant term at \( T = T_c \), the temperature-dependent contribution \( \propto (1 - T/T_c) \) in the square bracket may not be placed outside. Indeed, we obtain
\[
y(T) - y(T_c) = -b_1 b_2 c \delta^2 + \left[ (b_1 b_2 c \delta)^2 \right] \left[ \frac{3}{2} \delta^2 (1 - T/T_c) \right]^{1/2}
\]
\[
\approx 0.369 \delta^{1/2} (1 - T/T_c) : 1 - T/T_c \ll 10.5 \delta^3
\]
\[
\approx \sqrt{3 \zeta(2)^{1/3}} (1 - T/T_c) : 1 - T/T_c \gg 10.5 \delta^3.
\]

Noting \( y = (\Delta/T)^{1/2} \) and Eq. (53), we may approximate \( \Delta \) just below \( T_c \) as
\[
\Delta(T) - \Delta(T_c) = \left\{ 2.69 (1 - T/T_c) : 1 - T/T_c \ll 10.5 \delta^3 \right\}
\]
\[
\approx \sqrt{9 \delta^3 (1 - T/T_c)^{1/2} : 1 - T/T_c \gg 10.5 \delta^3}.
\]

Let us substitute Eqs. (52) and (53) into Eq. (49). We then find that \( n_0(T) \) grows as
\[
\frac{n_0}{n} = \left\{ \frac{0.369 \delta^{1/2} (1 - T/T_c)}{\sqrt{3 \zeta(2)^{1/3}} (1 - T/T_c)^{1/2}} : 1 - T/T_c \ll 10.5 \delta^3 \right\}.
\]

Equations (52), (53), (55), and (56) are the main results obtained from Eq. (49).

We turn our attention to other thermodynamic quantities. The chemical potential below \( T_c \) satisfies the Hugenholtz-Pines relation \( \mu_n(T) = -\Delta(T) \) and directly reflects the singularity of \( \Delta(T) \) near \( T_c \). On the other hand, \( \mu_n(T) \) in the normal state of \( T \geq 1 \) obeys
\[
\mu_n(T) = -\zeta(3)^2 \frac{T^{3/2}}{4 \pi} (T^{-1/2} - 1)^2.
\]

This can be shown from \( N = \frac{1}{\Delta} \sum \left[ e^{(s_0 + \Sigma - \mu_n)/T} - 1 \right] \) with the procedure of deriving the expansions of Eq. (22). Using Eqs. (52) and (53), we obtain the discontinuity \( \Delta \mu(T_c) \equiv \mu_n(T_c) - \mu_n(T_c) \) as
\[
\Delta \mu(T_c) = -\frac{4 \pi}{\zeta(2)^{1/2}} \delta^2 = -6.6 \delta^2.
\]

Next, with the procedure of deriving Eq. (22), the entropy just below \( T_c \) is calculated from Eq. (49) as
\[
\frac{S_n}{N} = \frac{5 \zeta(2)^{1/2} T^{3/2} - 3 \zeta(3)^2}{2 \zeta(2)^{1/2}} T^{1/2} \Delta.
\]

The corresponding normal-state expression for \( T \geq 1 \) is given by
\[
\frac{S_n}{N} = \frac{5 \zeta(2)^{1/2} T^{3/2} - 3 \zeta(3)^2}{8 \pi} (T^{-3/2} - 1)^2.
\]
Hence the discontinuity \( \Delta S(T_c) = S_n(T_c) - S_n(T_c) \) is found by using Eqs. (62) and (63) as
\[
\Delta S(T_c) = - \frac{6\pi}{\zeta(\frac{3}{2})^2/3} \delta^2 = -9.94 \delta^2.
\] (61)

It follows from Eqs. (58) and (65) that the specific heat \( C_s = T(\partial S_s/\partial T) \) just below \( T_c \) is given to the leading order by
\[
\frac{C_s}{N} = \frac{15\zeta(\frac{3}{2})}{4(\frac{3}{2})^2} T^{3/2} - \frac{3}{2} T^{3/2} \frac{d\Delta}{dT} = \frac{C_n}{N} + \left\{ \begin{array}{ll}
4.04 & : 1 - T/T_c < 10.5 \delta^3 \\
3 \sqrt{6\pi} \delta^{3/2} & : 1 - T/T_c \gg 10.5 \delta^3.
\end{array} \right.
\] (62)

It displays a divergent behavior \( C_s/N \sim 13.0 \delta^{3/2}(1 - T/T_c)^{-\frac{5}{3}} \) for \( 10.5 \delta^3 \ll 1 - T/T_c \ll 1 \).

Substituting Eq. (48c) into Eq. (43), \( p_s \) just below \( T_c \) is obtained as
\[
\frac{p_s}{n} = \frac{\Sigma}{2} \Delta \frac{n_0}{n} + \frac{\zeta(\frac{5}{2})}{\zeta(\frac{7}{2})} T^{5/2} - T^{3/2} \frac{\Delta}{T}.
\] (63)

The normal-state pressure of \( T \geq 1 \) can be calculated similarly to be
\[
\frac{p_n}{n} = \frac{\Sigma}{2} + \frac{\zeta(\frac{5}{2})}{\zeta(\frac{7}{2})} T^{5/2} - \frac{\zeta(\frac{5}{2})^2}{4\pi} T^{3/2} - 1^2.
\] (64)

Hence the discontinuity \( \Delta p(T_c) = p_s(T_c) - p_n(T_c) \) is obtained as
\[
\Delta p(T_c) = - \frac{4\pi}{\zeta(\frac{3}{2})^2/3} \delta^2 = -6.63 \delta^2.
\] (65)

It follows from Eqs. (53) and (55) as well as \( F(T, V, N) = -pV + \mu N \) that \( F_n(T_c; V, N) = F_n(T_c, V, N) \) is satisfied for the expression (62) up to the order \( \delta^2 \). Thus, Eq. (62) is indeed a correct expression of \( T_c \) of order \( \delta \).

We finally consider the superfluid density near \( T_c \). With the procedure of deriving Eq. (48), Eq. (55) is transformed into
\[
\frac{\rho_s}{mn} = 1 - T^{3/2} + \frac{4\sqrt{2\pi} T^{1/2}}{3\zeta(\frac{2}{3})} \Delta.
\] (66)

Substituting Eqs. (52) and (55) into Eq. (66), we obtain
\[
\frac{\Delta \rho_s(T_c)}{mn} = \frac{4\pi}{3\zeta(\frac{2}{3})^{1/3}} \delta = 1.16 \delta.
\] (67)

**C. Properties at \( T = 0 \)**

Physical properties at \( T = 0 \) are easily found from Eqs. (59) and (61-65) by dropping terms with the Bose distribution function. The leading-order expressions are summarized as follows:
\[
\frac{n_0(0)}{n} = 1 - \frac{8}{3\sqrt{\pi}} \delta^{3/2} = 1 - 1.50 \delta^{3/2},
\] (68a)
\[
\mu_s(0) = \Delta(0) = \frac{2\rho_s(0)}{n} = 2\zeta(\frac{3}{2})^{3/2} \delta = 3.79 \delta.
\] (68b)

**D. Numerical Results**

Figure 2 displays the specific heat \( C/N \) as a function of \( T/T_c \) for \( a_n^{1/3} = 0.01 \). The ideal-gas result \( n_0/n = \rho_s/nm \) is also plotted for comparison.

![FIG. 2: Specific heat \( C/N \) as a function of \( T/T_c \) for \( a_n^{1/3} = 0.01 \). The ideal-gas result is also plotted for comparison.](image)

![FIG. 3: Normalized condensate density \( n_0/n \) and superfluid density \( \rho_s/mn \) as a function of \( T/T_c \) for \( a_n^{1/3} = 0.01 \). The ideal-gas result is also plotted for comparison.](image)
upward from the ideal-gas result to show the limiting behavior \(T \lesssim T_c\).

Figure 3 plots \(n_0/n\) and \(\rho_s/nm\) as a function of \(T/T_c\) for \(\alpha^{1/3} = 0.01\) and 0. We observe that the finite interaction causes an enhancement of \(n_0/n\) and \(\rho_s/nm\) over the ideal-gas value at all temperatures. The enhancement is larger for \(\rho_s/nm\) than \(n_0/n\). The quantity \(n_0/n\) obeys Eq. (50) near \(T_c\) and develops continuously from 0 even with a finite interaction, whereas \(\rho_s/nm\) starts from a positive value at \(T_c\) as Eq. (57).

Figure 4 shows the chemical potential as a function of \(T/T_c\) for \(\alpha^{1/3} = 0.01\) and 0. With a finite interaction, the chemical potential displays a characteristic peak at \(T_c\) with a discontinuity, as shown explicitly by Eq. (58). It eventually approaches the value of Eq. (68b) as the temperature is lowered.

E. The HFB and Shohno theories

We now compare the above predictions of the conserving gapless mean-field theory with those of the HFB\(^{14,21,29,45}\) and Shohno\(^{22,29}\) theories. Although extensive theoretical studies have been carried out based on the latter theories, their predictions on the thermodynamic quantities seem not to have been clarified completely, especially near \(T_c\). We hence study them in detail with a special focus on the region \(T \lesssim T_c\). This will also help us to understand common features in the mean-field theories of the homogenous weakly interacting Bose gas. The transition temperature will be determined below in the same way as Eq. (62); the two comments below Eqs. (65) and (66) also apply to the present cases.

The equations to determine the equilibrium in the HFB theory are formally obtained from Eqs. (41) and (42) by a couple of modifications: (i) a sign change for the second term in the square bracket of Eq. (42); (ii) the expressions of \(\xi_k\) and \(E_k\). Indeed, they are given by

\[
\begin{align*}
n &= n_0 + \frac{1}{V} \sum_k \left( \frac{\xi_k}{E_k} \frac{1}{e^{E_k/T} - 1} + \frac{\xi_k - E_k}{2E_k} \right), \\
\Delta &= \frac{4\pi \hbar^2 a}{m} n_0 - \Gamma,
\end{align*}
\]

where \(\Gamma, \xi_k,\) and \(E_k\) are defined by

\[
\begin{align*}
\Gamma &= \frac{4\pi \hbar^2 a}{mV} \sum_k \left( \frac{\Delta}{E_k} \frac{1}{e^{E_k/T} - 1} + \frac{\Delta}{2E_k} \right), \\
\xi_k &= \varepsilon_k + \Delta + 2\Gamma, \quad E_k \equiv \sqrt{(\varepsilon_k + 2\Gamma)(\varepsilon_k + 2\Delta + 2\Gamma)},
\end{align*}
\]

with \(\varepsilon_k \equiv \hbar^2 k^2/(2m)\). The Shohno theory is obtained from Eqs. (69) and (71) by setting \(\Gamma = 0\).

Near \(T \sim T_0 = 1\) where \(\Delta\) and \(\Gamma\) are much smaller than \(T_0\), Eq. (69) is approximated to the leading order by

\[
\frac{n_0}{n} = 1 - T^{3/2} \left[ 1 - b_1 \left( \sqrt{\Gamma + \Delta} - \sqrt{\Gamma} \right) \right],
\]

with \(b_1 \equiv 2\pi \zeta(3/2)\) and \(c \equiv 2\zeta(3)^{2/3}\). These equations correspond to Eq. (10) and have been obtained with the procedure of deriving the expansions of Eq. (15). Note that Eq. (72) is also non-analytic in \(\Gamma\) and \(\Gamma + \Delta\). Using \(\Delta = c\delta(n_0/n - 1)\) from Eq. (69b), we next rewrite Eq. (72a) in terms of \(\Gamma\) and \(n_0/n\). We also introduce the dimensionless variables \(r, s, t\), and \(s\) through \(\sqrt{n_0/n} = b_1 \sqrt{c\delta} r, \sqrt{\Gamma} = b_1 c\delta s,\) and \(T = 1 + b_1^2 c\delta t\). Retaining terms of order \(\delta\), Eq. (72) is transformed into

\[
r^2 - r + \frac{3}{2} t = s, \quad s = \frac{-1 + \sqrt{1 + 4r}}{2}.
\]

Equation (72) yields

\[
f(r, t) \equiv r^4 - 2r^3 + (2 + 3t)r^2 - (2 + 3t)r + \frac{3}{4} (2 + 3t) = 0.
\]

It has a couple of solutions \(r_1, r_2 > 0\) for \(t \approx 0\) but no real solution for a large-enough \(t\). Thus, the transition temperature corresponds to the point where \(f = 0\) and \(\partial f / \partial r = 0\), which yields the critical values of \(t = 11/24\) and \(r = 3/4\). Thus, the transition temperature of the HFB theory for \(\delta \to 0\) is given by \(T_c^{\text{HFB}} = 1 + \Delta T_c^{\text{HFB}}\) with

\[
\Delta T_c^{\text{HFB}} = \frac{11\pi}{6\zeta(3)^{1/3}} \delta = 1.60\delta.
\]

The transition is clearly first order. The discontinuities of various thermodynamic quantities at \(T_c^{\text{HFB}}\) can be obtained with the procedure of Sec. 11\(\text{B}\) as

\[
\frac{n_0^{\text{HFB}}(T_c)}{n} = \frac{9\pi}{4\zeta(3)^{1/3}} \delta = 1.96\delta.
\]
\[ \Delta_{\text{HFB}}(T_c) = \frac{5\pi}{2\zeta(\frac{1}{2})} \delta^2 = 4.146^2, \quad (75c) \]

\[ \frac{\rho_{\text{HFB}}(T_c)}{m n} = \frac{139\pi}{60\zeta(\frac{1}{2})^4/3} \delta = 2.02\delta. \quad (75d) \]

Note that even \( n_0/n \) is discontinuous at \( T_c \) in the HFB theory.

The same analysis can be performed for the Shohno theory. We thereby obtain

\[ \Delta_{\text{Shohno}}(T_c) = \frac{2\pi}{3\zeta(\frac{1}{2})} \delta = 0.582\delta, \quad (76a) \]

\[ \frac{n_0^{\text{Shohno}}(T_c)}{n} = \frac{\pi}{\zeta(\frac{1}{2})} \delta = 0.873\delta, \quad (76b) \]

\[ \Delta_{\text{Shohno}}(T_c) = \frac{2\pi}{\zeta(\frac{1}{2}) \delta^2} = 3.31^2, \quad (76c) \]

\[ \frac{\rho_{\text{Shohno}}(T_c)}{m n} = \frac{5\pi}{3\zeta(\frac{1}{2})} \delta = 1.46\delta. \quad (76d) \]

Thus, even the Shohno theory predicts an enhancement of \( T_c \) over the ideal-gas value \( T_0 \).

As for the overall temperature dependences of various thermodynamic quantities, the HFB and Shohno theories both yield results qualitatively similar to those of the previous mean-field theory except the discontinuity of \( n_0 \) at \( T_c \). For example, the specific heat of the HFB and Shohno theories also display the divergent behavior of \((T_c - T)^{-1/2}\) just below \( T_c \). Due to a finite \( \Gamma \), the HFB theory generally predicts larger deviations from the ideal-gas results than the Shohno theory.

IV. HOMOGENEOUS GAS UNDER CONSTANT DENSITY

We finally study the homogeneous weakly interacting Bose gas under the complementary condition of constant pressure. Despite its fundamental importance as a subject of quantum statistical mechanics, the system seems to have been investigated only by Reatto and Straley based on the HFB and Shohno theories. Moreover, their main interest was on superfluid \(^4\)He so that the properties in the weak-coupling region remain essentially unexplored.

Let us introduce a dimensionless parameter \( \delta_p \) by

\[ \delta_p \equiv a \left( \frac{mp}{2\pi\hbar^2} \right)^{1/5}, \quad (77) \]

which completely characterizes the weak-coupling region of \( \delta_p \ll 1 \). The thermodynamic equilibrium of the condensed phase is determined by Eqs. 41 - 43. They yield the density \( n \), the condensate density \( n_0 \), and the pair potential \( \Delta \) as a function of \( p \) and \( T \). The prefactor \( A \) in Eqs. 41 - 43 may be rewritten conveniently as

\[ A = \frac{2n_c}{\sqrt{\pi \zeta(\frac{1}{2})}} \frac{T_0^{3/2}}{F_0^{5/2}}, \quad (78) \]

where \( n_c \) and \( T_0 \) are the critical density and the transition temperature of the ideal Bose gas, respectively. They are given in terms of \( p \) as \( n_c = \left[ mp/2\pi\hbar^2 \zeta(\frac{5}{2}) \right] \zeta(\frac{1}{2})/\zeta(\frac{5}{2}) \) and \( T_0 = (2\pi\hbar^2/m)^{3/2} [p/\zeta(\frac{3}{2})]^{3/5} \). The equations for the normal state are obtained from Eqs. 41, 43, and 44 by setting \( \Delta = n_0 = 0 \) and \( E = \xi = \epsilon + S_n - \mu_n \); they yield \( n, \mu_n, \) and \( S_n \) as a function of \( p \) and \( T \). The transition temperature \( T_c \) is then determined by the thermodynamic condition \( \mu_n(T_c, p) = \mu_n(T_c, p) \) appropriate under constant pressure. The specific heat per particle \( C_p \) may be calculated from the results on \( S \) by numerical integrations. In the following, we will adopt the units in which \( n_c = T_0 = 1 \) and neglect the cutoff-dependent term in Eq. 42 as was done in the case of constant density.

To investigate the properties near \( T_c \) (\( \sim 1 \)) in more detail, we make use of the asymptotic expansions of Eqs. 45. Equations 41 and 42 with Eq. 45 enable us to express \( n_0 \) and \( n \) in terms of \( T \) and \( \Delta \) as \( n_0 = \Delta/c' \delta_p - b_1 T \Delta^{1/2} \) and \( n = T^{3/2} + \Delta/c' \delta_p - 2b_1 T \Delta^{1/2} \) with \( c' \equiv 2\zeta(\frac{3}{2})/\zeta(\frac{3}{2})^{1/5} = 4.93 \). Substituting them into it, Eq. 46 becomes a nonlinear equation for \( \Delta \) as

\[ \frac{b_1''}{2c' \delta_p} \Delta^2 - \left( \frac{7b_1 b_1''}{2} - b_1'' \right) T \Delta^{3/2} \]

\[ + \left( b_1'' T^{3/2} + 4b_1 b_1'' T^{2} \delta_p \right) \Delta - 4b_1 b_1'' c'/T^{5/2} \delta_p \Delta^{1/2} \]

\[ + T^{5/2} + b_1'' c'/T - 1 = 0. \quad (79) \]

Thus, the equation is non-analytic in \( \Delta \) and completely different from the one in the Landau theory of second-order transition. It is convenient to rewrite \( T \) in Eq. 70 as \( T = 1 - \frac{2b_1'' \delta_p + t}{b_1'' \delta_p + t} = 1 - 3.84b_1 + t^2 \). where \( t \) is a parameter appropriate to describe the region \( T \sim 1 \).

Then Eq. 79 can be solved analytically by expanding \( \Delta \) as \( \Delta = \Delta_2(t) \delta_p^2 + \Delta_3(t) \delta_p^3 + \cdots \). The expression for \( \Delta_2(t) \) is obtained as

\[ \Delta_2(t) = \sqrt{2b_1 c' + \sqrt{\left(2b_1 c'\right)^2 + \frac{9b_1'' c'^2}{10} - \frac{5}{2b_1'' t}}} \cdot \quad (80a) \]

It hence follows that a superfluid solution exists for \( t < t_c = (2b_1'' c')^2 + 9b_1'' c'^2/10 \) = 103. The quantity \( \Delta_2(t) \) may be expressed in terms of \( \Delta \) and \( \delta_p(t) \). A similar consideration for the normal state leads to a nonlinear equation for \( \Sigma - \mu \). Expanding \( \Sigma - \mu = \Sigma_2(t) \delta_p^2 + \Sigma_3(t) \delta_p^3 + \cdots \), \( \Sigma_2(t) \) is found to satisfy

\[ \sqrt{\Sigma_2(t)} = -\sqrt{2b_1 c' + \sqrt{2(b_1 c')^2 - \frac{9b_1'' c'^2}{10} + \frac{5}{2b_1'' t}}}. \quad (80b) \]
It has a real solution $\Sigma_2$ for $t \geq t_n = 18(b'_c c')^2 / 50 = 33.1$.

From $t_s > t_n$, we realize that the superfluid transition is first order with a metastable region extending over $t_n \leq t \leq t_s$. The transition temperature $T_c$ can also be expressed as

$$T_c = 1 - 3.84\delta_p + t_c\delta_p^2.$$  \hspace{1cm} (81)

Thus, $T_c$ becomes smaller than $T_0 = 1$ to the leading order in $\delta_p$. This behavior is opposite to the case of constant volume where $T_c$ increases as a function of the dimensionless parameter $a\nu^{1/3}$. Indeed, the effect of the weak repulsive interaction is completely different between the volume-fixed and pressure-fixed cases. In the former case, a finite interaction suppresses the density fluctuation so that it works favorably for the phase coherence over the system, thereby leading to an enhancement of $T_c$. In the latter case, on the other hand, the interaction lowers the particle density to decrease $T_c$. The value of the prefactor 3.84 is almost certainly correct, in contrast to the volume-fixed case where it seems still controversial.

We turn our attention to $t_c$ of Eq. (81) which includes all the higher-order contributions. It is found that $t_c$ has a rather large $\delta_p$ dependence, due partly to the large values of the numerical constants appearing in the equations, e.g., $t_s = 103$. It decreases from $t_c(\delta_p \rightarrow 0) = t_s = 103$ down to 98.6, 96.9, and 95.7 at $\delta_p = 5.0 \times 10^{-4}$, $1.0 \times 10^{-3}$, and $1.5 \times 10^{-3}$, respectively. The contributions from $\Delta_3$ and $\Sigma_3$ are essential to produce the results, which agree excellently with the exact numerical results of using Eqs. 111-113 for $T \sim 1$. Discontinuities in the thermodynamic quantities at $T_c$ are found to be all of the order of $\delta_p^2$ in accordance with the tiny metastable region.

Let us move onto the overall temperature dependences of various thermodynamic quantities. Figure 5 plots specific heat $C_p$ over $0.6T_c \leq T \leq 1.2T_c$ for $\delta_p = 0.001$ and 0.005. A remarkable enhancement of $C_p$ near $T_c$ is clearly seen. Indeed, the curves show a divergent behavior $\propto (T - T_c)^{-1/2}$ on both sides near $T_c$. It is completely different from the discontinuous behavior predicted by the Landau theory of second-order transition and caused by the non-analytic nature of the order-parameter expansion near $T_c$. The sharp heat absorption/emission near $T_c$ may be realized in terms of the proximity to the ideal Bose gas under constant pressure which sud-
denly falls into the ground state of volume zero below $T_c$. The weak repulsive interaction weakens the singularity of the ideal Bose gas at $T = T_0$ over a finite range close to $T_c$. This sharp absorption/emission of heat near $T_c$ in the present system is in qualitative agreement with the observation on $^4$He. Figure 6 shows the normalized condensate density $n_0/n$ as a function of temperature, where a steep change just below $T_c$ can also be seen clearly. Although not plotted here, the normalized superfluid density $\rho_s(T)/mn(T)$ is almost indistinguishable in the present scale from $n_0(T)/n(T)$ for both $\delta_p = 0.001$ and 0.005. Figure 7 displays temperature dependence of the chemical potential $\mu$. The curves flatten out rapidly below $T_c$ reflecting proximity to the ground state. Finally, Fig. 8 plots the particle density $n$ as a function of temperature for $\delta_p = 0.001$ and 0.005. Since the superfluid component contributes less to the pressure than the normal component in the weak-coupling region, a constant pressure can only be sustained at lower temperatures by increasing the particle density. Thus, $n(T)$ increases monotonically as $T$ is lowered from $T_c$. The leading-order expression of $n(0)$ is given by $n(0)/n_c = \left[3 \zeta(2)/\zeta(3)\right]^{1/2}/2 \mu_{\Delta}^{1/2}$, implying a smaller enhancement of $n(0)$ for a stronger interaction. In this respect, it is worth pointing out that $n(T)$ of superfluid $^4$He displays a maximum at $T_c$. Whether $n(0)/n(T_c)$ may be reduced beyond 1 or not in the strong-coupling region remains a challenging problem to be clarified theoretically.

V. SUMMARY

We have constructed a mean-field theory for Bose-Einstein condensates. The basic equations to determine the equilibrium are given by Eqs. (14), (15), (24), and (30). They are applicable to general non-uniform systems such as the trapped atomic gases with or without vortices. The present theory has a manifest advantage over the HFB and Sholmo theories that it simultaneously satisfies the Hugenholtz-Pines theorem and various conservation laws. It will be useful in clarifying both equilibrium and dynamical properties of condensed Bose gases over the whole temperature range. The conserving gapless theory is expected to provide at least a qualitative description of weakly interacting BEC. Especially, it will shed a new light on the temperature dependences of the collective modes in BEC. It may also form a starting point for a unified description of BEC over the whole interaction strengths from the trapped weakly interacting atomic gases to superfluid $^4$He.

The theory is then applied to a homogeneous weakly interacting Bose gas with $s$-wave scattering length $a$ under constant density $n$ in Sec. III and under constant pressure $p$ in Sec. IV. The order-parameter expansion near $T_c$ is found not of the Landau-Ginzburg type but non-analytic by nature due to the divergence of the Bose distribution function at zero energy, as shown explicitly in Sec. IIIB. This non-analyticity makes the superfluid transition first-order and also brings unique temperature dependences of various thermodynamic quantities near $T_c$ which are quite different from those of the Landau theory of second-order transition. The transition temperature $T_c$ under constant $n$ is found to increase from the ideal Bose gas value $T_0$ as $T_c/T_0 = 1 + 2.33a_{\Delta}^{1/3}/T_0$, whereas it decreases under constant pressure as $T_c/T_0 = 1 - 3.84a_{\Delta}^{1/2}/\sqrt{\pi T_0}$ We have also clarified overall temperature dependences of basic thermodynamic quantities in Secs. IIIID and IV. These predictions are then compared with those of the HFB,14,31,29,43 and Sholmo22,29 theories in Sec. IIIE. Those theories also predict a first-order transition and an enhancement of $T_c$.

We finally comment on the first-order superfluid transition of the present mean-field theory. As mentioned above, it is a feature inherent in the mean-field theories of BEC stemming from the non-analyticity of the Bose distribution function at zero energy. However, it is in contradiction to the observation of superfluid $^4$He where the transition is continuous. It has been pointed out by Reatto and Straley29 that the mean-field transition would be continuous if the change of the single-particle dispersion at $T_c$ were from $k$ to $k^{1/2}$ with $\epsilon < \frac{3}{2}$ ($k$: wave number). The behavior $k^{1/2}$ with $\epsilon < \frac{3}{2}$ above $T_c$ may only be possible by including correlations and/or fluctuations. Thus, we encounter the question of whether the correlations and/or fluctuations are essential even in the limit $a \to 0$ to transform the nature of the superfluid transition. If not so, the transition is expected to change its character from first-order into continuous at an intermediate value of $a$. Thus, the predictions of the mean-field theory raise the questions on: (i) the relative importance of the single-particle and collective excitations in BEC as a function of the interaction strength; (ii) the role of the single-particle excitations in superfluid $^4$He above and below $T_c$. It is worth reminding that the transition of the ideal Bose gas under constant pressure is strongly first-order. Hence it may not be so unreasonable to expect that the first-order transition persists into the region of a finite interaction.

Thus far, microscopic theoretical studies on condensed Bose systems seem to have been carried out separately in two limiting cases with completely different approaches: (a) the weak-coupling regime where certain model Hamiltonians have been investigated based on the field theory22,29 (b) the strong coupling regime where interests have been focused on describing superfluid $^4$He quantitatively based on some variational wave functions62,63,64 lattice-gas models which can be mapped onto spin systems65 and quantum Monte-Carlo calculations.66 We hence need systematic investigations based on a model Hamiltonian from weak- to strong-coupling regimes, which may provide us more profound understanding on condensed Bose systems and shed a new light on the nature of the still mysterious lambda transition of superfluid $^4$He.65
APPENDIX A: FEYNMAN RULES IN NAMBU SPACE

The bare perturbation expansion of the condensed Bose systems is usually carried out with respect to the condensate wave function \( \Psi(\mathbf{r}) \) and the non-interacting Green's function:

\[
G^{(0)}(\mathbf{r}_1, \mathbf{r}_2) = -(T_\tau \phi(r_1) \phi^\dagger(r_2))_0. \tag{A1}
\]

The anomalous (i.e., off-diagonal) Green's function is not necessary before the renormalization, and we have well-established Feynman rules for this purpose. We will show that the same rules can be used with a slight modification to the perturbation expansion in terms of the Nambu matrix of Eq. (3). This extension will be performed in exactly the same way as the extension from the normal to the perturbation expansion in terms of the Nambu matrix of Eq. (3). This extension will be performed in exactly the same way as the extension from the normal to the superconducting Fermi systems.

Let us consider the following term in the interaction:

\[
H^{(3)} = U_{11'} \left( \Psi^*_1 \phi^\dagger_1 \phi^\dagger_{1'} \phi^\dagger_{1'} + \phi^\dagger_1 \phi^\dagger_{1'} \phi^\dagger_{1'} \Psi_1 \right),
\]

where \( U_{11'} = U(r_1 - r'_1) \), \( \phi_1 \equiv \phi(r_1) \), etc., and summations over the repeated indices are implied. Using the normal-ordering operator \( N \), we first rewrite Eq. (A2) as

\[
H^{(3)} = U_{11'} N \left( \Psi^*_1 \phi^\dagger_1 \phi^\dagger_{1'} + \phi^\dagger_1 \Psi^*_1 \phi^\dagger_{1'} \right). \tag{A3a}
\]

With the operator \( N \) in front, Eq. (A3a) is further transformed into

\[
H^{(3)} = U_{11'} N \left( \frac{1}{2} \Psi^*_1 \phi^\dagger_1 \phi^\dagger_{1'} + \frac{1}{2} \phi^\dagger_1 \phi^\dagger_{1'} \Psi^*_1 \right), \tag{A3b}
\]

where \( \tilde{\phi} \) and \( \tilde{\Psi} \) are the spinors of Eq. (2). Comparing Eqs. (A3a) and (A3b), we observe the following correspondence:

\[
\phi^\dagger_i \leftrightarrow \tilde{\phi}^\dagger_1, \quad \Psi^*_i \leftrightarrow \tilde{\Psi}^\dagger_1, \quad \phi^\dagger_1 \phi^\dagger_{1'} \leftrightarrow \frac{1}{2} \phi^\dagger_1 \phi^\dagger_{1'} \tilde{\phi}^\dagger_1 \tilde{\phi}^\dagger_{1'}, \quad \text{etc.} \tag{A4}
\]

Let us perform a perturbation expansion in the imaginary time domain with respect to (A3b). We then include \( r_i \) in the index \( i \), i.e., \( i \equiv r_i \tau_i \) and \( i' \equiv r'_i \tau_i \). Consider an \( n \)-th-order term in the expansion and take a contraction of \( \phi^\dagger_i \) with \( \frac{1}{2} \phi^\dagger_1 \phi^\dagger_{1'} \) and \( \phi^\dagger_{1'} \phi^\dagger_{1''} \) with \( \frac{1}{2} \phi^\dagger_1 \phi^\dagger_{1'} \). We then find that \( \phi^\dagger_i \) and \( \phi^\dagger_{1'} \) contribute equivalently to the contraction, as shown easily by writing it down with respect to \( \phi_i, \phi^\dagger_i, \phi_{1'}, \) and \( \phi^\dagger_{1'} \); the statement is valid even if we formally retain the anomalous averages. Because of this fact, we can introduce the rule: Contract \( \phi^\dagger_i \) only with \( \phi^\dagger_{1'} \) in \( \frac{1}{2} \phi^\dagger_1 \phi^\dagger_{1'} \) and multiply the contribution by 2. This yields \( \phi^\dagger_i (T_\tau N \phi^\dagger_{1'} \phi^\dagger_{1''})_0 \), where \( N \) is effective only when \( i \) and \( j \) belong to the same interaction line according to the definition in Eq. (A3). Note \( \langle T_\tau \phi^\dagger_1 \phi^\dagger_{1'} \rangle_0 = -\tau_3 G_{ji}^{(0)} \) as realized from Eq. (3). The rule allows us to perform a perturbation expansion in Nambu space by using only the Feynman diagrams for \( G^{(0)} \).

The following two points should be supplemented: (a) A factor \( \frac{1}{2} \) remains uncancelled for each closed particle line, due to the fact that we have to fix the starting pair \( \phi^\dagger_i \phi^\dagger_{1'} \) for each closed line. (b) The contraction of \( \phi^\dagger_i \) with the last \( \phi^\dagger_k \) in the closed particle line may be transformed as

\[
\frac{1}{2} \langle T_\tau N \phi^\dagger_k \hat{A}_{ki} \phi^\dagger_1 \rangle_0 = \frac{1}{2} \text{Tr} \hat{A}_{ki} \langle T_\tau N \phi^\dagger_1 \phi^\dagger_1 \rangle_0, \tag{A5}
\]

where \( \hat{A}_{ki} \) is a Nambu matrix composed of the contractions connecting \( k \) with \( i \). (c) As for the open line starting from \( \phi^\dagger_1 \tilde{\Psi}_i \) and ending at \( \Phi_{1'} \tilde{\phi}^\dagger_{1''} \), the two factors \( \frac{1}{2} \) remain uncancelled. These rules are valid even after including the interactions other than Eq. (A3).

In summary, we can carry out a perturbation expansion in Nambu space by modifying the Feynman rules for \( G^{(0)}, \Psi, \) and \( \Psi^* \) as follows: (i) \( G^{(0)} \rightarrow \tilde{\Psi}^\dagger_i \tilde{G}_{ij}, \Psi_i \rightarrow \frac{1}{2} \tilde{\Psi}_i, \) and \( \Psi^*_i \rightarrow \frac{1}{2} \tilde{\Psi}^\dagger_i \); (ii) \( \frac{1}{2} \text{Tr} \) for every closed particle line. Note that the operator \( N \) in \( \langle T_\tau N \phi^\dagger_1 \phi^\dagger_1 \rangle_0 \) transforms into the matrix of Eq. (A3) in the frequency space.

Let us write down the contributions of the diagrams in Fig. (1) based on the above rules with \( G^{(0)} \rightarrow \tilde{G} \). This yields \( \Phi_{\text{HFB}} \). We then modify it slightly as described below Eq. (11a). We thereby obtain \( \Phi \) of Eq. (11a).

APPENDIX B: CONSERVATION LAWS

It is shown that the \( \Phi \) derivative approximation defined by Eqs. (7) and (10) automatically satisfies various conservation laws.

1. Definitions

Since we work in the real-time domain, we need modifications of various definitions. The Green’s function is now defined by

\[
\tilde{G}(1, 2) \equiv -\frac{i}{\hbar} \tau_3 (T_\tau \tilde{G}(1, 2)), \tag{B1}
\]

with \( 1 \equiv r t_1 \). It obeys the equation of motion:

\[
\frac{i \hbar}{\partial t_1} \tilde{G}(1, 1') - \tau_3 K_1 \tilde{G}(1, 1') = \delta(1, 1') + \tilde{S}(1, 2) \tilde{G}(2, 1'), \tag{B2a}
\]
or equivalently,
\[-i\hbar \frac{\partial \hat{G}(1,1')}{\partial t_1} - K_1 \hat{G}(1,1') \hat{\mathbf{r}}_3 = \hat{1} \delta(1,1') + \hat{G}(1,2) \hat{\Sigma}(2,1').\]  
(B2b)

Here \(K_1\) is given by Eq. (15), and integration over the barred index 2 is implied. Next, the condensate wave function satisfies
\[i\hbar \frac{\partial}{\partial t_1} \hat{\Psi}(1) - K_1 \hat{\Psi}(1) = \hat{r}_3 \hat{\eta}(1),\]  
(B2c)
or equivalently,
\[-i\hbar \frac{\partial}{\partial t_1} \tilde{\hat{\Psi}}(1) - K_1 \tilde{\hat{\Psi}}(1) = \hat{r}_3 \tilde{\hat{\eta}}(1).\]  
(B2d)

Here \(\hat{\Psi}\) is given in Eq. (23), and \(\hat{\eta}(1)\) denotes
\[\hat{\eta}(1) \equiv \begin{bmatrix} \eta(1) \\ \eta^*(1) \end{bmatrix} .\]  
(B3)
The key quantities in Eqs. (B2a) are \(\hat{\Sigma}\) and \(\hat{\eta}\). In the \(\Phi\)-derivative approximation adopted here, they are determined from a functional \(\Phi = \Phi(\hat{G}, \Psi, \Psi^*)\) by
\[\hat{\Sigma}(1,1') = -2i \frac{\delta \Phi}{\delta \hat{G}(1',1)} ,\]  
(B4a)
\[\eta(1) = \hbar \frac{\delta \Phi}{\delta \Psi^*(1)}.\]  
(B4b)

Note that this \(\Phi\) is different in definition from those of Baym and Hohenberg and Martin by factor \(i\), i.e., \(\Phi = i \Phi_{\text{Baym}} = i \Phi_{\text{HM}}\). The present definition has an advantage that \(\Phi\) becomes real within the mean-field approximation. A comment is also necessary on Eq. (B5). When \(t_2 = t_1\), the operator \(\hat{\phi}^1\) in \(\hat{G}(1,2)\) should be placed to the left of \(\phi\) by definition. This procedure is in accordance with the treatment on the equal-time operators in the calculation of \(\hat{\Phi}\). Put it another way, the equal time implies \(t_2 = t_1^+\) for the \((11)\) component of \(\hat{G}\) and \(t_2 = t_1^-\) for the \((22)\) component. Thus, \(t_2\) is not exactly equal to \(t_1\) for the diagonal elements of \(\hat{G}\).

2. Identities

With Eq. (B4), we can prove several identities by exactly following the argument of Baym.

Suppose we perform the gauge transformation:
\[
\begin{align*}
\hat{G}(1,2) & \rightarrow e^{i \chi(1) \hat{\mathbf{r}}_3} \hat{G}(1,2) e^{-i \chi(2) \hat{\mathbf{r}}_3} , \\
\Psi(1) & \rightarrow e^{i \chi(1)} \Psi(1) ,
\end{align*}
\]  
(B5)

where \(\chi(1)\) is an arbitrary real function. The corresponding variations in \(\hat{G}\) and \(\Psi\) are given to the leading order by
\[
\begin{align*}
\delta \hat{G}(1,2) & = i [\chi(1) \hat{r}_3 \hat{G}(1,2) - \hat{G}(1,2) \chi(2) \hat{r}_3] , \\
\delta \Psi(1) & = i \chi(1) \Psi(1) ,
\end{align*}
\]  
(B6)

respectively. However, \(\Phi\) is clearly invariant under Eq. (B5), i.e., \(\delta \Phi = 0\). This yields
\[i\hbar \frac{\partial}{\partial t_1} \hat{\Sigma}(1,2) \delta \hat{G}(2,1) + \delta \Psi^*(1) \eta(1) + \delta \Psi(1) \eta^*(1) = 0 .\]  
(B7)

Substituting Eq. (B6) into Eq. (B7) and recalling \(\chi(1)\) is arbitrary, we obtain
\[i\hbar \frac{\partial}{\partial t_1} \tilde{\hat{\Psi}}(1) \delta \hat{G}(2,1) - \tilde{\hat{\Sigma}}(1,2) \delta \hat{G}(2,1) - \frac{i}{\hbar} \delta \tilde{\hat{\Psi}}(1) \tilde{\hat{\eta}}(1) = 0 ,\]  
(B8)

with \(\delta \tilde{\hat{\Psi}} = (\Psi^* \hat{\Psi})\).

We next consider the Galilean transformation:
\[
\begin{align*}
\hat{G}(1,2) & \rightarrow \hat{G}(\mathbf{r}_1 + \mathbf{R}(t_1), t_1; \mathbf{r}_2 + \mathbf{R}(t_2), t_2) , \\
\hat{\Psi}(1) & \rightarrow \hat{\Psi}(\mathbf{r}_1 + \mathbf{R}(t_1), t_1) ,
\end{align*}
\]  
(B9)

The corresponding leading-order variations in \(\hat{G}\) and \(\Psi\) are given by
\[
\begin{align*}
\delta \hat{G}(1,2) & = [\mathbf{R}(t_1) \cdot \nabla_1 + \mathbf{R}(t_2) \cdot \nabla_2] \hat{G}(1,2) , \\
\delta \hat{\Psi}(1) & = \mathbf{R}(t_1) \cdot \nabla_1 \hat{\Psi}(1) .
\end{align*}
\]  
(B10)

However, \(\Phi\) remains invariant since it is a quantity obtained by integrations over all the space-time variables. We hence conclude that Eq. (B7) holds also in this case. Substituting Eq. (B10) into Eq. (B7) and recalling \(\mathbf{R}(t)\) is arbitrary, we obtain
\[\int S(1) d\mathbf{r}_1 = 0 ,\]  
(B11)

with
\[S(1) \equiv \frac{1}{4} (\nabla_1 - \nabla_{1'}) \{i \hbar \text{Tr} [\hat{G}(1,2) \hat{\Sigma}(2,1') - \hat{\Sigma}(1,2)]
\times \hat{G}(2,1') - 2 \hat{\tilde{\Psi}}(1') \hat{\tilde{\eta}}(1) \} \bigg|_{1'} .\]  
(B12)

Here terms with \(\nabla_1 \hat{\Sigma}(1,2)\) and \(\nabla_1 \hat{\eta}(1)\) have been obtained through integrations by parts.

We finally consider the “rubber-clock” transformation of Baym \(t \rightarrow \theta(t) \equiv t + f(t)\) with \(f(\pm \infty) = 0\). It yields
\[
\begin{align*}
\hat{G}(1,2) & \rightarrow \left( \frac{d \theta_1}{d t_1} \right)^{1/4} \hat{G}(\mathbf{r}_1 \theta_1, \mathbf{r}_2 \theta_2) \left( \frac{d \theta_2}{d t_2} \right)^{1/4} , \\
\hat{\Psi}(1) & \rightarrow \left( \frac{d \theta_1}{d t_1} \right)^{1/4} \hat{\Psi}(\mathbf{r}_1 \theta_1) ,
\end{align*}
\]  
(B13)

The factor \((d \theta/dt)^{1/4}\) compensates the Jacobian for \(t \rightarrow \theta\), thereby making the integration of \(H_{\text{int}}(t)\) over \(t\) invariant in form through the change of variables. The corresponding leading-order variations in \(\hat{G}\) and \(\hat{\Psi}\) are given by
\[
\begin{align*}
\delta \hat{G}(1,2) & = \left( \frac{f_1 + f_2}{4} f_1 \frac{\partial}{\partial t_1} + f_2 \frac{\partial}{\partial t_2} \right) \hat{G}(1,2) , \\
\delta \hat{\Psi}(1) & = \left( \frac{f_1}{4} f_1 \frac{\partial}{\partial t_1} \right) \hat{\Psi}(1) ,
\end{align*}
\]  
(B14)
with $f_j \equiv f(t_j)$. However, $\Phi$ remains invariant. Hence Eq. (B7) holds also in this case. Substituting Eq. (B4) into Eq. (B7) and recalling $f(t)$ is arbitrary, we obtain the third identity:

$$\frac{d\langle H_{\text{int}}\rangle_1}{dt_1} = \frac{1}{2} \int dr_1 \frac{\partial}{\partial t_1} \left\{ \langle h \text{Tr}[\hat{G}(1, 2)\hat{\Sigma}(2, 1') + \hat{\Sigma}(1')\hat{G}(1, 2)] \times \hat{\Sigma}(2, 1) + \hat{\Psi}^\dagger(1)\eta(1') + \eta^\dagger(1')\hat{\Psi}(1) \rangle \right\}_{1' = 1},$$

(B15)

where $\langle H_{\text{int}}\rangle_1$ is defined by

$$\langle H_{\text{int}}\rangle_1 = \frac{1}{8} \int dr_1 \left\{ i\hbar \text{Tr}[\hat{G}(1, 2)\hat{\Sigma}(2, 1) + \hat{\Sigma}(1')\hat{G}(1, 2)] + \hat{\Psi}^\dagger(1)\eta(1) + \eta^\dagger(1')\hat{\Psi}(1) \right\}.$$  

(B16)

Equation (B16) indeed corresponds to the interaction energy of the system. This can be checked as follows: (i) write down the equations of motion for $\phi$ and $\Psi$ in terms of the field operators and the condensate wave function; (ii) construct the interaction energy by adding those equations appropriately; and (iii) transform the one-particle energy in the equation by using Eq. (B2). Equations (B8), (B11), and (B15) are the basic identities to be used below.

3. Conservation laws

Let us operate $\frac{i}{\hbar} \text{Tr}\hat{\gamma}_3$, $-\frac{i}{\hbar} \text{Tr}\hat{\gamma}_3$, and $-\frac{i}{\hbar} \hat{\Psi}^\dagger(1)$ to Eqs. (B2a), (B2b), and (B2c), respectively. Adding the resulting three equations, setting $1' = 1$, and noting Eq. (B8), we obtain the particle conservation law as

$$\frac{\partial n(1)}{\partial t_1} + \nabla_1 j(1) = 0,$$

(B17)

where $n(1)$ and $j(1)$ are defined by

$$n(1) = \rho(1, 1),$$

(B18)

$$j(1) = -\frac{i\hbar}{2m} (\nabla_1 - \nabla_{1'})\rho(1, 1')|_{1' = 1},$$

(B19)

with

$$\rho(1, 1') \equiv \langle \phi^\dagger(1')\phi(1) \rangle + \Psi(1)\Psi^*(1').$$

(B20)

This $\rho(1, 1')$ is the one-body density matrix appearing in the evaluation of every one-particle operator.

To obtain the momentum conservation law, we operate $-\frac{i\hbar}{2m} \text{Tr}(\nabla_1 - \nabla_{1'})$, $\frac{i\hbar}{2m} \text{Tr}(\nabla_1 - \nabla_{1'})$, and $-\frac{i}{\hbar} \hat{\Psi}^\dagger(1)\hat{\gamma}_3\nabla_1$ to Eqs. (B2a), (B2b), and (B2c), respectively. We also multiply Eq. (B2b) from the right by $\frac{1}{\hbar m} \hat{\gamma}_3\nabla_1^\dagger\hat{\Psi}(1)$. Adding the four equations and setting $1' = 1$, we obtain

$$\frac{\partial j(1)}{\partial t_1} + \frac{n(1)}{m} \nabla_1 V(1) + \frac{1}{m} \nabla_1 \cdot \Pi(1) = \frac{1}{m} S(1).$$

(B21)

Here $j(1)$, $n(1)$, and $S(1)$ are given by Eqs. (B19), (B18), and (B22), respectively, and $\Pi(1)$ is a tensor defined by

$$\Pi_{\alpha\beta}(1) = -\frac{\hbar^2}{4m} (\nabla_{1\alpha} - \nabla_{1'\alpha})(\nabla_{1\beta} - \nabla_{1'\beta})\rho(1, 1')|_{1' = 1}.$$  

(B22)

Integrating Eq. (B21) over $r_1$ and noting Eq. (B15), we obtain the conservation law for the total momentum as

$$\frac{d\langle H_{\text{int}}\rangle_1}{dt_1} = -\int dr_1 K_1 \frac{\partial}{\partial t_1} \rho(r_1 t_1, r_1' t_1)|_{r_1' = r_1}.$$  

(B24)

with $\rho(1, 1')$ defined by Eq. (B20). When $K$ has no time dependence as given by Eq. (6), Eq. (B24) directly leads to $\langle K + H_{\text{int}} \rangle = \text{constant}$. Following Kadanoff and Baym, we may alternatively consider $V$ as a small time-dependent external field and trace the time variation of the internal energy $\langle K^{(0)} + H_{\text{int}} \rangle$, where $K^{(0)} = -\frac{\hbar^2}{2m} \nabla^2$. Using Eq. (B17) and performing integration by parts with respect to $r_1$, we obtain

$$\frac{d\langle K^{(0)} + H_{\text{int}}\rangle_1}{dt_1} = -\int j(1) \cdot \nabla_1 V(1) \, dr_1.$$  

(B25)

Thus, we have seen that the conservation laws are automatically obeyed as Eq. (B15), (B23), and (B25) in the $\Phi$ derivative approximation of Eq. (B4).

APPENDIX C: THE IRK THEORY

It will be shown that the thermodynamic functional presented by Ivanov, Riek, and Knoll (IRK) leads to exactly the same thermodynamic properties for the weakly interacting Bose gases as the present theory. The IRK self-energy $\hat{\Sigma}^{\text{(IRK)}}$ is calculated from Eq. (14) by Eq. (6). The result can be written as

$$\hat{\Sigma}^{\text{(IRK)}}(r, r') = \left[ \begin{array}{cc} \Sigma(r, r') & -\Delta^{\text{(IRK)}}(r, r') \\ \Delta^{\text{(IRK)}}^*(r, r') & -\Sigma^*(r, r') \end{array} \right],$$

(C1)

where $\Sigma$ is given by Eq. (14), and $\Delta^{\text{(IRK)}}$ denotes

$$\Delta^{\text{(IRK)}}(r, r') = U(r - r')\rho^{\text{(IRK)}}(r, r'),$$

(C2)

with

$$\rho^{\text{(IRK)}}(r, r') = \Psi(r)\Psi^*(r') - \langle \phi(r)\phi(r') \rangle^{\text{(IRK)}}.$$  

(C3)
The minus sign in front of $\Delta^{\text{IRK}}$ in Eq. (C1) has been introduced to make the coefficient $\Delta^{\text{IRK}}_{\vec{k}}$ for the homogeneous system positive at low temperatures, in accordance with the definition of $\Delta$ in Eq. (14). Next, the equation for $\Psi(r)$ is obtained from the thermodynamic functional $\Omega^{\text{IRK}}$ by $\partial\Omega^{\text{IRK}}/\partial\Psi(r) = 0$. It is given by Eq. (10) with the replacement: $\Delta = \Delta^{\text{IRK}}$.

In a way parallel to Eqs. (18) and (24), let us introduce the Hamiltonian:

$$\hat{H}^{\text{IRK}}(r, r') \equiv \hat{\tau}_3 K \delta(r-r') + \hat{\Sigma}^{\text{IRK}}(r, r'),$$

and construct the eigenvalue problem as

$$\int \hat{H}^{\text{IRK}}(r, r') \hat{u}_\nu^{\text{IRK}}(r') \text{d}r' = \hat{u}_\nu^{\text{IRK}}(r) E_\nu \hat{\tau}_3,$$

where $\hat{u}_\nu^{\text{IRK}}(r)$ is defined by

$$\hat{u}_\nu^{\text{IRK}}(r) = \begin{bmatrix} u_\nu(r) & v_\nu(r) \\ v_\nu^*(r) & u_\nu^*(r) \end{bmatrix}.$$ (C6)

The sign of $v_\nu^*(r)$ is chosen so that the coefficient $v_\nu$ of the homogeneous system is positive, in accordance with the definition of $v_\nu^*(r)$ in Eq. (2a). The corresponding Green’s function $\hat{G}^{\text{IRK}}$ is obtained from Eq. (20) with the replacement $\hat{u}_\nu \rightarrow \hat{u}_\nu^{\text{IRK}}$. Noting Eqs. (20a) and (20b), we now conclude that $\langle \phi(r)|\phi(r')\rangle^{\text{IRK}}$ in Eq. (C6) satisfies $-\langle \phi(r)|\phi(r')\rangle^{\text{IRK}} = \langle \phi(r)|\phi(r')\rangle^{\text{IRK}}$, which implies $\Delta^{\text{IRK}} = \Delta$. Thus, the equations to determine the equilibrium are exactly the same between the present theory and the IRK theory. Finally, one can show that the equilibrium thermodynamic potential of the IRK theory is also given by Eq. (31). Thus, the two functionals (11a) and (12) yield exactly the same thermodynamic properties on BEC.

APPENDIX D: NON-HERMITIAN EIGENVALUE PROBLEM

In this Appendix we study possible origins of the non-Hermitian eigenvalue problem in BEC. It is shown that we have to treat the non-Hermitian matrix of Eq. (24) necessarily if we impose the two requirements: (i) the quasiparticle field obey the Bose statistics; (ii) the quasiparticle eigenstates be obtained by diagonalizing a matrix.

Let us introduce the quasiparticle field $\gamma_\nu$ through

$$\begin{bmatrix} \phi_r \\ -\phi_r^\dagger \end{bmatrix} = \sum_\nu \begin{bmatrix} u_{r\nu} & -v_{r\nu} \\ v_{r\nu}^* & u_{r\nu}^* \end{bmatrix} \begin{bmatrix} \gamma_\nu \\ -\gamma_\nu^\dagger \end{bmatrix},$$

where $\nu$ distinguishes quasiparticle eigenstates, and $\phi_r = \phi(r)$, $u_{r\nu} = u_{\nu}(r)$, etc. Equation (D1) may be written symbolically in a compact form as

$$\vec{\phi} = \hat{u}\vec{\gamma},$$

with

$$\vec{\phi} = \begin{bmatrix} \phi_r \\ \phi_r^\dagger \\ \vdots \\ -\phi_r \\ -\phi_r^\dagger \end{bmatrix}, \quad \hat{u} = \begin{bmatrix} u_{r\nu} & -v_{r\nu} \\ v_{r\nu}^* & u_{r\nu}^* \end{bmatrix}, \quad \vec{\gamma} = \begin{bmatrix} \gamma_\nu \\ \gamma_\nu^\dagger \\ \vdots \\ -\gamma_\nu \\ -\gamma_\nu^\dagger \end{bmatrix}.$$ (D3)

We now impose the condition that $\gamma_\nu$ as well as $\phi_r$ obey the Bose statistics. This implies

$$\hat{\tau}_3 = [\vec{\phi}, \vec{\phi}^\dagger] = \hat{u}[\vec{\gamma}, \vec{\gamma}^\dagger] \hat{u}^\dagger = \hat{u}\hat{\tau}_3 \hat{u}^\dagger,$$

where $\hat{\tau}_3$ is an infinite matrix defined by

$$\hat{\tau}_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

with $1$ and $0$ denoting the unit and the zero matrices, respectively. We also require that $\hat{u}$ be composed of eigenstates of a matrix $\hat{H}$ as

$$\hat{H}\hat{u} = \hat{u}\hat{E},$$

where $\hat{E}$ is a real diagonal matrix. Multiplying Eq. (D7) by $\hat{u}^{-1} = \hat{\tau}_3 \hat{u}^\dagger \hat{\tau}_3$ from the left, we obtain

$$\hat{\tau}_3 \hat{u}^\dagger \hat{\tau}_3 \hat{H}\hat{u} = \hat{E}.\quad$$ (D8a)

We next take the Hermitian conjugate of Eq. (D8a) and multiply the resulting equation by $\hat{\tau}_3$ from both sides; this yields

$$\hat{\tau}_3 \hat{u}^\dagger \hat{H}^\dagger \hat{\tau}_3 \hat{u} = \hat{E}.\quad$$ (D8b)

Subtracting Eq. (D8b) from Eq. (D8a) and multiplying the resulting equation by $\hat{\tau}_3 \hat{u}^\dagger$ from the left and the right, respectively, we obtain

$$\hat{H}^\dagger = \hat{\tau}_3 \hat{H} \hat{\tau}_3.$$ (D9)

Thus, $\hat{H}$ is necessarily non-Hermitian with the property (D9).

APPENDIX E: DERIVING EQUGS. (31) AND (32)

We here derive expressions of the equilibrium thermodynamic potential (31) and the entropy (32).

Using Eqs. (18) and (28), the logarithmic term in Eq. (4) can be transformed as

$$L = \frac{T}{2} \sum_n \text{Tr} \hat{1}(z_n) \ln(\hat{\tau}_3 K + \hat{\Sigma} - z_n \hat{1})$$

$$= \frac{1}{2} \int \text{d}r \int \frac{dz}{2\pi i} e^{ia_0} n(z) \sum_\nu |u_{\nu}(r)|^2 \left[ \ln(E_\nu + z) + \ln(z - E_\nu) \right]$$

$$+ \ln(z - E_\nu) - |v_{\nu}(r)|^2 \left[ \ln(E_\nu + z) + \ln(-z - E_\nu) \right],$$

(E1)
with \( n(z) = 1/(e^{z/T} - 1) \). Here we have used the standard procedure to change the summation over \( n \) into a contour integral, with the replacements \( e^{z_n/0} \to n(z)e^{z_0+} \) and \( e^{-z_n/0} \to -n(-z)e^{-z_0} \) in the matrix \( \hat{I}(z_n) \) of Eq. (3). Contour \( C \) consists of two parallel lines running along the imaginary axis as shown in Fig. 25.4 of Ref. [69], which can be deformed into contour \( C' \) in the same figure along the real axis. Performing integration by parts in terms of \( z \) and collecting residues within \( C' \), we obtain

\[
L = \sum_{\nu} \left[ T \ln(1 - e^{-E_\nu/T}) - E_\nu \int |\nu(r)|^2 dr \right].
\]

(E2)

Next, we rewrite \( \Phi \) of Eq. (11a) by using Eqs. (13)-(15) as

\[
\Phi = \frac{1}{4} \text{Tr} \int d\tau \int d\tau' \hat{\Sigma}(\tau, \tau') \left[ -T \sum_n \hat{G}(\tau', r; z_n) \hat{I}(z_n) \right. \\
\left. + \hat{\gamma}_3 \hat{\Psi}(\tau') \hat{\Psi}(r) \right].
\]

(E3)

Finally, the first integral in Eq. (4) is transformed with Eq. (10) into an expression without \( K \). Substituting the result together with Eqs. (19) and (20) into Eq. (4), we arrive at Eq. (31).

We next derive Eq. (32) by closely following the procedure of Ref. [51]. We first transform all the summations over \( n \) in Eq. (4) into contour integrals of using \( n(z) \). With the properties \( \delta \Omega/\delta \Psi^* = 0 \) and \( \delta \Omega/\delta G = 0 \), the differentiation \( \partial \Omega/\partial T \) need be carried out only with respect to the explicit \( T \) dependence in \( n(z) \). The term from \( \Phi \) cancels that from the second term in the square bracket of Eq. (4). The remaining term is \( L \) of Eq. (12), whose explicit \( T \) dependence is transformed into the first term in Eq. (15). We hence obtain Eq. (32).

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