Conserving and gapless Hartree-Fock-Bogoliubov theory for the three-dimensional dilute Bose gas

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The excitation spectrum for the three-dimensional Bose gas in the Bose-Einstein condensation phase is calculated nonperturbatively with the modified Hartree-Fock-Bogoliubov theory, which is both conserving and gapless. From improved Φ-derivable theory, the diagrams needed to preserve the Ward-Takahashi identity are re-summed in a systematic and nonperturbative way. It is valid up to the critical temperature where the dispersion relation of the low-energy excitation spectrum changes from linear to quadratic. Because including the higher-order fluctuation, the results show significant improvement on the calculation of the shift of critical temperature with other conserving and gapless theories.

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I. INTRODUCTION

Since Einstein and Bose's first proposal of Bose-Einstein condensation (BEC) and experimental realization of it with alkali atoms [1–3], weakly interacting dilute Bose gas has attracted significant attentions [4].

The description of BEC at zero temperature began from Bogoliubov [5] and quantum loop corrections to energy density were calculated up to two loops [6–11] at low temperature. The self-consistent Hartree-Fock-Bogoliubov (HFB) approximation was used but it gave a gapped spectrum [12–14], violating the Hugenholtz-Pines theorem [8] or the Goldstone theorem [15], which results from the spontaneous symmetry breaking of $U(1)$. Popov theory neglects the anomalous average and gets a gapless spectrum [16,17]. But the anomalous average is not negligible at the broken phase. To correctly describe the BEC at high temperature, we need a theory to be both conserving (consistent with the conservation laws) and gapless [12,14,18]. The many-body T matrix has been used to obtain a modified Popov approximation [19]. However, this approach yields the same critical temperature as that of ideal gas and the Hugenholz-Pines theorem is not always satisfied (as noted in [4]). An improved Popov approximation based on a many-body T-matrix approximation was developed [20,21] but its main application is in low-dimensional systems. Recently, conserving and gapless approximation has been developed by Kita with a modified Luttinger-Ward functional [22] and Cooper *et al.* with a leading-order auxiliary field approximation [23]. Their results coincides with the Bogoliubov theory at zero temperature with weak coupling and predicts a second-order phase transition.

It is of significant importance to develop a conserving and gapless theory beyond mean-field level to better calculate the excitation spectrum and the critical temperature. First, the dispersion of elementary excitations relates to the critical velocity of the superfluid according to Landau's criterion [24]. Besides, it has been shown that the critical temperature (T_c) of weakly interacting Bose gas in three dimensions is positively shifted from that of ideal gas (T_0) proportional to the scattering length a: $\frac{T_c-T_0}{T_0} = cn^{1/3}a$ [25–29]. The accurate determination of c by lattice simulations [30,31] shows $c \approx 1.29$, while Kita and Cooper's theory from the broken phase gives $c = 2.33$ [22,23]. A nonperturbative theory beyond mean-field level is needed to correctly describe the broken phase near T_c. And, when interaction is strong, the exact result may differ from mean-field theory even at low temperature due to strong fluctuation effects.

In this work we presents a modified Hartree-Fock-Bogoliubov (MHFB) approximation which is conserving and gapless and is beyond mean-field level. The method is based on the two-particle irreducible (2PI) Φ-derivable theory in which the full propagator serves as an infinite set of varitional parameters. It was first formulated by Luttinger and Ward [32], and later shown by Baym [33] that Φ-derivable theory naturally obeys the conservation laws and later Cornwall, Jackiw, and Tomboulis generalized it to relativistic field theories [34]. However, the Φ-derivable approximation does not necessarily guarantee the Goldstone theorem when applied to the Bosonic system with spontaneous symmetry breaking. Indeed, within the 2PI truncated functional approach, the solution of Eq. (4) is gapped. Reference [22] found a modified functional with a gapless solution, however it contains some terms which are not 2PI. Later, Van Hees and Knoll developed an improved Φ-derivable theory which preserve the Ward-Takahashi identity (WTI) by approximating the 1PI functional with the 2PI functional [35]. We take Van Hees and Knoll's method which is based on the 2PI functional approach to systematically add the infinite series of diagrams needed to preserve WTI and the same result can be equivalently obtained from the Schwinger-Dyson equation approach [36–38].

The paper is organized as following. In Sec. II the Φ-derivable theory is introduced to develop the modified HFB theory. Numerical results including the excitation spectrum and the shift of T_c are given in Sec. III. Finally, we give a summary. In the Appendix an alternative approach based on the Schwinger-Dyson equation is provided which gets the same result with the Φ-derivable theory.

II. MODIFIED HFB THEORY

For Bose gas, the grand-canonical partition function can be written with imaginary time path integral [4]

$$Z[J,B] = \int D[\psi,\psi^*]e^{-S[\psi^*,\psi]-\int d(1)J_i\psi_i-\frac{1}{2}\int d(12)B_{ij}\psi_i\psi_j}, \quad (1)$$

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where the action (in dimensionless units) is

$$S[\psi,\psi^*] = \int_0^\beta d\tau \int d^dx \left(\psi^*[\partial_\tau - \mu + \nabla^2]\psi + \frac{g}{2}\psi^*\psi^*\psi\psi\right) \tag{2}$$

and $g = 8\pi a$, where a is the scattering length. $\beta = \frac{1}{T}$. ψ_1, ψ_2 represent ψ^*, ψ. $d(1)$ means $d\tau d^dx$ and J_i, B_{ij} are auxiliary sources which will be set to zero at last.

The 2PI (two-particle irreducible) functional $\Gamma[\varphi,G]$ is defined by the double Legendre transformation and can be written in the form

$$\Gamma[\varphi,G] = S[\varphi_i] + \tfrac{1}{2}\mathrm{Tr}\{D^{-1}(G-D)\} + \tfrac{1}{2}\mathrm{Tr}\ln G^{-1} + \Phi[\varphi,G], \tag{3}$$

where $D_{ij}^{-1} = \frac{\delta^2 S[\varphi_i]}{\delta\varphi_i\varphi_j}$ and $\varphi_i = \langle\psi_i\rangle$. G_{ij} is the Green function $G_{ij} = \langle\psi_i\psi_j\rangle_c = \langle\psi_i\psi_j\rangle - \langle\psi_i\rangle\langle\psi_j\rangle$. $\Phi[\varphi,G]$ is the sum of all 2PI vacuum diagrams.

$\Phi[\varphi,G]$ can be expanded to the n loop and we get an n loop Φ-derivable approximation. Then we can get the truncated φ and G^{tr} by solving

$$\frac{\delta\Gamma[\varphi,G^{\mathrm{tr}}]}{\delta\varphi_i} = 0, \quad \frac{\delta\Gamma[\varphi,G^{\mathrm{tr}}]}{\delta G_{ij}^{\mathrm{tr}}} = 0. \tag{4}$$

Including the simplest diagrams (Hartree-Fock approximation)

$$\Phi[\varphi,G] = \frac{g}{2}\int d(1)[G_{11}(x,x)G_{22}(x,x) + 2G_{12}(x,x)G_{21}(x,x)]. \tag{5}$$

For homogeneous gas we define $\upsilon = \varphi_1 = \varphi_2$. Then $G_{ij}(x,y) = G_{ij}(x-y)$. x means $(\tau,\vec{x})$.

Then from (4) we get the shift equation and gap equation:

$$\mu = g\upsilon^2 + gG_{11}^{\mathrm{tr}}(0) + 2gG_{12}^{\mathrm{tr}}(0), \tag{6}$$

$$\Gamma_{\mathrm{tr}}^{(2)} = \begin{pmatrix} \Sigma_{11}^{\mathrm{tr}} & -i\omega_n - \mu + \Sigma_{12}^{\mathrm{tr}} + k^2 \\ i\omega_n - \mu + \Sigma_{12}^{\mathrm{tr}} + k^2 & \Sigma_{11}^{\mathrm{tr}} \end{pmatrix}. \tag{7}$$

The equation is written after Fourier transformation $G_{ij}(x-y) = \frac{1}{V\beta}\sum_{\omega_n,k} G_{ij}(\omega_n,\vec{k})e^{-i\omega_n\tau + i\vec{k}\cdot(\vec{x}-\vec{y})}$; $\Gamma_{\mathrm{tr}}^{(2)} = G^{\mathrm{tr}-1}$. ω_n is the Matsubara frequency $\omega_n = \frac{2\pi n}{\beta}$. And we define $\Sigma_{11}^{\mathrm{tr}} = g\upsilon^2 + gG_{11}^{\mathrm{tr}}(0)$, $\Sigma_{12}^{\mathrm{tr}} = 2g\upsilon^2 + 2gG_{12}^{\mathrm{tr}}(0)$. Due to the symmetry we have $G_{12}^{\mathrm{tr}}(0) = G_{21}^{\mathrm{tr}}(0)$, $G_{11}^{\mathrm{tr}}(0) = G_{22}^{\mathrm{tr}}(0)$.

We define $\mu_R = \mu - \Sigma_{12}^{\mathrm{tr}}$. $\mu_R, \Sigma_{11}^{\mathrm{tr}}$ can be solved self-consistently with G^{tr} which is the inverse of Γ^{tr}:

$$G^{\mathrm{tr}} = \frac{1}{(i\omega_n)^2 - \omega_k^2}\begin{pmatrix} \Sigma_{11}^{\mathrm{tr}} & i\omega_n - k^2 + \mu_R \\ -i\omega_n - k^2 + \mu_R & \Sigma_{11}^{\mathrm{tr}} \end{pmatrix} \tag{8}$$

so

$$\Sigma_{11}^{\mathrm{tr}} = g\upsilon^2 + \frac{g}{V\beta}\sum_{\omega_n,k}\frac{\Sigma_{11}^{\mathrm{tr}}}{(i\omega_n)^2 - \omega_k^2}, \qquad \mu_R = -2g\upsilon^2 + \Sigma_{11}^{\mathrm{tr}}, \tag{9}$$

where $\omega_k = \sqrt{(k^2 - \mu_R)^2 - (\Sigma_{11}^{\mathrm{tr}})^2}$.

In three dimensions $\alpha_0 = \frac{1}{V\beta}\sum_{\omega_n,k}\frac{1}{(i\omega_n)^2 - \omega_k^2} = -\frac{1}{V}\sum_k (\frac{1}{\omega_k}\frac{1}{e^{\beta\omega_k}-1} + \frac{1}{2\omega_k})$ has the ultraviolet divergence due to the double counting problem, which arises because we use the pseudopotential. The pseudopotential has already effectively incorporated in the first term of the Born series the information of the higher-order terms [39]. To avoid this problem, the vacuum terms should be subtracted: $\alpha_R = \alpha_0 + \frac{1}{V}\sum_k \frac{1}{2k^2}$. Equation (9) after renormalization is

$$\Sigma_{11}^{\mathrm{tr}} = g\upsilon^2 - g\frac{\Sigma_{11}^{\mathrm{tr}}}{V}\sum_k\left(\frac{1}{\omega_k}\frac{1}{e^{\beta\omega_k}-1} + \frac{1}{2\omega_k} - \frac{1}{2k^2}\right). \tag{10}$$

The density $n = -\frac{1}{\beta V}\frac{\partial\Gamma}{\partial\mu}$ can be calculated from (3):

$$n = \upsilon^2 + G_{12}^{\mathrm{tr}}(0) \tag{11}$$

and

$$G_{12}^{\mathrm{tr}}(0) = \frac{1}{V\beta}\sum_{\omega_n,k}\frac{i\omega_n - k^2 + \mu_R}{(i\omega_n)^2 - \omega_k^2} = \frac{1}{V}\sum_k\left(\frac{k^2-\mu_R}{\omega_k}\frac{1}{e^{\beta\omega_k}-1} + \frac{k^2-\mu_R-\omega_k}{2\omega_k}\right). \tag{12}$$

We can get υ and G^{tr} from n, a, and T with Eqs. (9)–(12).

WTI is not necessarily preserved by Φ-derivable approximations when truncation is made and the solution of (4) is not gapless. An improved Φ-derivable theory was developed to systematically add the necessary diagrams to preserve WTI and thus satisfy the Goldstone theorem. We use $\Gamma[\varphi,G^{\mathrm{tr}}]$ to approximate the 1PI effective action:

$$\Gamma[\varphi] = \Gamma[\varphi,G^{\mathrm{tr}}(\varphi)], \tag{13}$$

with $G^{\mathrm{tr}}(\varphi)$ defined by $\frac{\delta\Gamma[\varphi,G^{\mathrm{tr}}]}{\delta G_{ij}^{\mathrm{tr}}} = 0$. The equivalence of the 2PI functional and the 1PI functional at the exact level was shown in Ref. [34].

Because $\Gamma[\varphi,G^{\mathrm{tr}}(\varphi)]$ conserves the symmetry [as in (3)], the IPI effective action remains unchanged under the transformation of $U(1)$ symmetry. The Green function defined by the inverse of

$$\Gamma^{(2)} = \frac{\delta^2\Gamma^{\mathrm{tr}}[\varphi]}{\delta\varphi_i\delta\varphi_j} \tag{14}$$

will be gapless. It is easy to show that

$$\Gamma^{(2)} = \Gamma_{\mathrm{tr}}^{(2)} + \frac{\delta^2\Gamma[\varphi,G^{\mathrm{tr}}]}{\delta\varphi_i(x)\delta G_{mn}^{\mathrm{tr}}}\frac{\delta G_{mn}^{\mathrm{tr}}}{\delta\varphi_j(y)}. \tag{15}$$

$\frac{\delta G_{mn}^{\mathrm{tr}}}{\delta\varphi_j(y)}$ can be obtained by taking the derivative of

$$\int d(2')\Gamma_{\mathrm{tr};ij'}^{(2)}G_{j'j}^{\mathrm{tr}} = \delta_{ij}. \tag{16}$$

By defining $\Lambda_{j'jm}^{\mathrm{tr}} = \frac{\delta G_{j'j}^{\mathrm{tr}}}{\delta\varphi_m}$, $\Gamma_{ijm}^{(3)} = \frac{\delta\Gamma_{\mathrm{tr};ij}^{(2)}}{\delta\varphi_m}$; we get

$$\Lambda_{j'jm}^{\mathrm{tr}} = -\int d(1',2')\Gamma_{im'm}^{(3)}G_{j'i}^{\mathrm{tr}}G_{m'j}^{\mathrm{tr}}. \tag{17}$$

$\Gamma^{(3)}_{ijm}$ can be gotten by taking the derivative of (7). These equations are actually the Bethe-Salpeter equation to solve $\Lambda^{\rm tr}_{j'jm}$.

In the level of HFB, we can get the modified HFB approximation:

$$\begin{aligned}
\Gamma^{(2)}_{11}(k) &= \Sigma^{\rm tr}_{11} + g\upsilon\Lambda^{\rm tr}_{221}(k) + 2g\upsilon\Lambda^{\rm tr}_{121}(k),\\
\Gamma^{(2)}_{12}(k) &= -i\omega_n - \mu_R + k^2 + g\upsilon\Lambda^{\rm tr}_{222}(k) + 2g\upsilon\Lambda^{\rm tr}_{122}(k),\\
\Gamma^{(2)}_{21}(k) &= i\omega_n - \mu_R + k^2 + g\upsilon\Lambda^{\rm tr}_{111}(k) + 2g\upsilon\Lambda^{\rm tr}_{121}(k),\\
\Gamma^{(2)}_{22}(k) &= \Sigma^{\rm tr}_{11} + g\upsilon\Lambda^{\rm tr}_{112}(k) + 2g\upsilon\Lambda^{\rm tr}_{122}(k),
\end{aligned} \tag{18}$$

where $\Lambda^{\rm tr}_{mnl}(k)$ is the Fourier transformation of $\Lambda^{\rm tr}_{mnl}(x,x,y) = \frac{\delta G^{\rm tr}_{mn}(x,x)}{\delta\varphi_l(y)}$. The latter can be solved by the Bethe-Salpeter equation (17):

$$\begin{aligned}
\Lambda^{\rm tr}_{mnl}(k) = {}& \Lambda^{\rm tr}_{lll}(k)I_{m\bar{l},\bar{l}n}(k) + \Lambda^{\rm tr}_{\bar{l}\bar{l}l}(k)I_{ml,ln}(k)\\
&+ \Lambda^{\rm tr}_{\bar{l}ll}(k)[2I_{ml,\bar{l}n}(k) + 2I_{m\bar{l},ln}(k)]\\
&+ 2\upsilon[I_{ml,\bar{l}n}(k) + I_{m\bar{l},ln}(k) + I_{m\bar{l},\bar{l}n}(k)],
\end{aligned} \tag{19}$$

where $\bar{l}$ is defined as $\delta_{l\bar{l}} = 0$ and

$$I_{mn,m'n'}(k) = -\frac{1}{V\beta}\sum_{\omega_{n1},k_1} G^{\rm tr}_{mn}(k_1+k)G^{\rm tr}_{m'n'}(k_1). \tag{20}$$

Again due to the double counting, $I_{12,21}$ and $I_{21,12}$ have ultraviolet divergences. They should be renormalized by subtracting vacuum diagrams:

$$\begin{aligned}
I^R_{12,21} &= -\left[\frac{1}{V\beta}\sum_{\omega_{n1},k_1} G^{\rm tr}_{12}(k_1+k)G^{\rm tr}_{21}(k_1) - Vac\right],\\
Vac &= \frac{1}{V}\sum_k \frac{1}{2k^2}.
\end{aligned} \tag{21}$$

Solve these linear equations and we can get the corrections to the self-energy. The corrections are the re-summation of the infinite series of diagrams (as shown in Fig. 1).

The Green function is the inverse of $\Gamma^{(2)}$. By analytic continuation $i\omega_n \to \Omega + i\varepsilon$, the retarded Green function G^R is gotten and the spectral weight function is

$$\rho(k,\Omega) = -2\,{\rm Im}\,G^R(k,\Omega). \tag{22}$$

III. NUMERICAL RESULTS

We solve the gap equation numerically and the result is shown in Fig. 2. The equation ceases to have a solution at T_c, which is the end point of the broken phase and is actually the critical point of a second-order phase transition. υ^2 is not exactly equal to the condensation number n_0 and needs corrections to get the exact n_0 just like $G^{\rm tr}$ needs corrections to get the exact Green function.

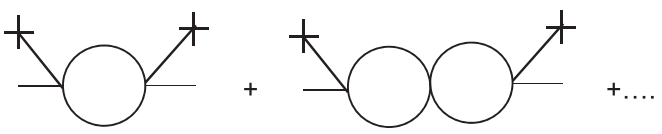

FIG. 1. The corrections to the self-energy is the re-summation of the infinite series of diagrams. The propagator in the diagrams are the gapped HFB ones but the final propagator after re-summation is gapless.

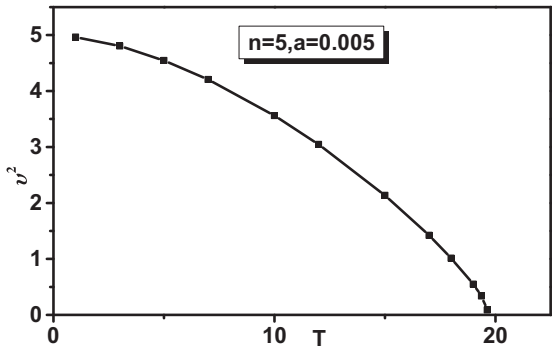

FIG. 2. υ^2-T for HFB theory when $n = 5$, $a = 0.005$, $T_0 = 19.3716$, $T_c = 19.635$. At T_c, $\upsilon^2 = 0.086$.

The spectral weight of quasiparticle is plotted in Fig. 3. The quasiparticle peak is broadened and the quasiparticle has finite lift time caused by the fluctuation effect.

At low temperature, the result of the modified HFB shows discrepancy with Popov theory and Cooper and Kita theory when interaction is strong, though it coincides with those theories at the weakly interacting limit at low temperature. It has been shown that in one dimension, as the interaction becomes large, the MHFB shows significant difference with Bogoliubov theory and is in very good agreement with the exact result at zero temperature [37]. So we expect systems in three dimensions which are less fluctuated than in one dimension, MHFB will also give quite an accurate result. From Fig. 4 it is obvious that at low temperature MHFB gives modifications to Popov theory while Kita and Cooper's theories are close to Popov theory, which can be tested in further experiments with strong interaction.

T_c is the end of the broken phase and actually at this point the linear dispersion of phonon spectrum disappears and the excitation spectrum becomes $\omega = k^2$, which indicates that this is the critical point of a second-order phase transition. By linear fit we show that T_c has a positive shift in comparison with the

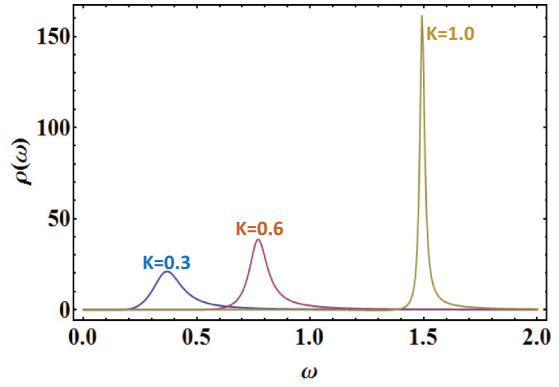

FIG. 3. (Color online) The spectral weight for $k = 0.3$, 0.6, 1 when $n = 5$, $a = 0.005$, $T = 10$. It is clear there is damping of the quasiparticle.

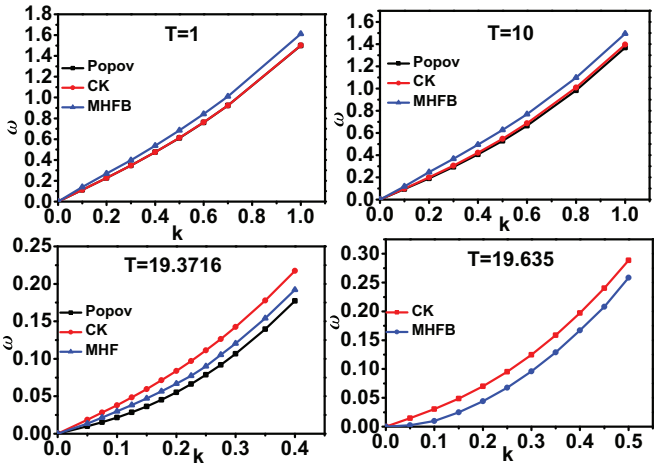

FIG. 4. (Color online) The excitation spectrum by Popov theory, Cooper-Kita theory, and modified HFB when $n = 5$, $a = 0.005$ for different temperatures; $T_0 = 19.3716$, $T_c = 19.635$. Kita and Cooper's theories get the same excitation spectrum. At $T = 1$, Cooper and Kita theory is very close to Popov theory.

ideal gas with coefficient $c = 1.59$ as shown in Fig. 5, while Kita and Cooper theory get $c = 2.33$.

IV. CONCLUSION

In conclusion, we calculate the excitation spectrum of BEC nonperturbatively with modified Hartree-Fock-Bogoliubov theory, which is developed by both the Φ-derivable theory and the Dyson-Schwinger theory. Our method is both conserving and gapless and is valid at the whole temperature regime up to critical temperature. Our theory predicts a second-order phase transition with a increased critical temperature compared with ideal gas $\frac{T_c - T_0}{T_0} = 1.59 n^{1/3} a$. It is different from Popov and Kita and Cooper theory at low temperature when interaction is strong and it significantly differs from Kita and Cooper theory near T_c . The damping of the quasiparticle is obtained in our theory while the quasiparticle in Popov, Kita, and Cooper theory has infinite lifetime because of the missing of the higher order diagrams. Modified HFB is the simplest improved Φ-derivable theory. However, the improved Φ-derivable theory can be generalized to higher order.

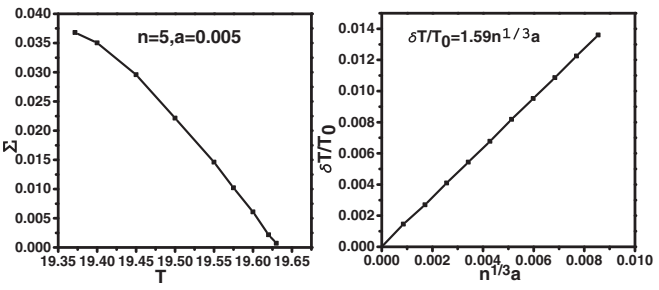

FIG. 5. (a) The Σ-T where Σ is fitted by $\omega = \sqrt{k^4 + 2\Sigma k^2}$. It is clear that the dispersion of energy spectrum changes to quadratic at T_c, $n = 5$, $a = 0.005$. (b) The linear fit of $\frac{T_c - T_0}{T_0} = c n^{1/3} a$. We get $c = 1.59$ with $R^2 = 0.99998$.

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APPENDIX

1. Dyson-Schwinger approach

At the level of HFB, the same result can be obtained with the 1PI Dyson-Schwinger approach instead of the 2PI Φ-derivable theory.

The generating functional is defined as

$$W[J^*, J] = -\ln \mathcal{Z}[J^*, J], \tag{A1}$$

where

$$\mathcal{Z}[J^*, J] = \int \mathcal{D}[\psi^*, \psi] e^{-(S[\psi^*,\psi] + J^*\psi + J\psi^*)}. \tag{A2}$$

By the derivatives of the generating functional

$$\varphi_m(\mathbf{x}, \tau) = \frac{\delta W[J^*, J]}{\delta J_m(\mathbf{x}, \tau)}. \tag{A3}$$

Successive derivatives generate Green function

$$G_{mn}(x, y) = -\frac{\delta^2 W}{\delta J_m(x) \delta J_n(y)}. \tag{A4}$$

The 1PI effective action is defined by the Legendre transformation

$$\Gamma[\varphi^*, \varphi] = W[J^*, J] - J^*\varphi - J\varphi^*. \tag{A5}$$

Then

$$\frac{\delta \Gamma[\varphi^*, \varphi]}{\delta \varphi_m(\mathbf{x}, \tau)} = -J_m(\mathbf{x}, \tau). \tag{A6}$$

It is easily proven that

$$\sum_i \int dz G_{mi}(x, z) \Gamma_{in}(z, y) = \delta_{mn} \delta(x - y), \tag{A7}$$

$$\Gamma_{in}(z, y) = \frac{\delta^2 \Gamma[\varphi^*, \varphi]}{\delta \varphi_i \delta \varphi_n(\mathbf{x}, \tau)}. \tag{A8}$$

The following identity:

$$\int \mathcal{D}[\psi^*, \psi] \frac{\delta}{\delta \psi_i(x)} e^{-(S[\psi^*,\psi] + J^*\psi + J\psi^*)} = 0, \tag{A9}$$

leads to Dyson-Schwinger equations:

$$\begin{aligned} (\partial_\tau - \nabla^2 - \mu)\varphi_2 + \langle \psi_1 \psi_2 \psi_2 \rangle + J_1 = 0, \\ (-\partial_\tau - \nabla^2 - \mu)\varphi_1 + \langle \psi_1 \psi_1 \psi_2 \rangle + J_2 = 0, \end{aligned} \tag{A10}$$

$$\begin{aligned} \langle \psi_1 \psi_2 \psi_2 \rangle = \langle \psi_1 \psi_2 \psi_2 \rangle_c + 2\varphi_2 \langle \psi_1 \psi_2 \rangle_c + \varphi_1 \langle \psi_2 \psi_2 \rangle_c \\ + \varphi_1 \varphi_2^2, \end{aligned} \tag{A11}$$

where $\langle \cdots \rangle_c$ means connected correlation functions. Preserving only up to two-point correlation functions yields

$$\begin{aligned} (\partial_\tau - \nabla^2 - \mu)\varphi_2 + \varphi_1 \varphi_2^2 + \varphi_1 G_{22}^{\mathrm{tr}} + 2\varphi_2 G_{12}^{\mathrm{tr}} + J_1 = 0, \\ (-\partial_\tau - \nabla^2 - \mu)\varphi_1 + \varphi_1^2 \varphi_2 + \varphi_2 G_{11}^{\mathrm{tr}} + 2\varphi_1 G_{12}^{\mathrm{tr}} + J_2 = 0. \end{aligned} \tag{A12}$$

By

$$\Gamma_{ij}(z,y) = \frac{\delta^2\Gamma[\varphi^*,\varphi]}{\delta\varphi_i\delta\varphi_j(\mathbf{x},\tau)} = -\frac{\delta J_i(x)}{\delta\varphi_j(y)} \tag{A13}$$

and do not consider the dependence of $G^{\rm tr}$ on φ, we get

$$\begin{aligned}
\Gamma^{\rm tr}_{11}(x,y) &= \left(\varphi_2^2 + G^{\rm tr}_{22}\right)\delta(x-y),\\
\Gamma^{\rm tr}_{22}(x,y) &= \left(\varphi_1^2 + G^{\rm tr}_{11}\right)\delta(x-y),\\
\Gamma^{\rm tr}_{12}(x,y) &= \left(\partial_\tau - \nabla^2_{\mathbf{x}} - \mu + 2\varphi_1\varphi_2 + 2G^{\rm tr}_{12}\right)\delta(x-y),\\
\Gamma^{\rm tr}_{21}(x,y) &= \left(-\partial_\tau - \nabla^2_{\mathbf{x}} - \mu + 2\varphi_1\varphi_2 + 2G^{\rm tr}_{12}\right)\delta(x-y).
\end{aligned} \tag{A14}$$

These are equivalent to (4) and form the HFB approximation.

By keeping source terms here and keeping the derivative of $G^{\rm tr}(\varphi)$ by φ, MHFB is obtained:

$$\begin{aligned}
\Gamma_{11}(x,y) &= \Gamma^{\rm tr}_{11}(x,y) + \varphi_1\Lambda^{\rm tr}_{221}(x,y) + 2\varphi_2\Lambda^{\rm tr}_{121}(x,y),\\
\Gamma_{22}(x,y) &= \Gamma^{\rm tr}_{22}(x,y) + \varphi_2\Lambda^{\rm tr}_{112}(x,y) + 2\varphi_1\Lambda^{\rm tr}_{122}(x,y),\\
\Gamma_{12}(x,y) &= \Gamma^{\rm tr}_{12}(x,y) + \varphi_1\Lambda^{\rm tr}_{222}(x,y) + 2\varphi_2\Lambda^{\rm tr}_{122}(x,y),\\
\Gamma_{21}(x,y) &= \Gamma^{\rm tr}_{21}(x,y) + \varphi_2\Lambda^{\rm tr}_{111}(x,y) + 2\varphi_1\Lambda^{\rm tr}_{121}(x,y),
\end{aligned} \tag{A15}$$

where

$$\Lambda^{\rm tr}_{mnl}(x,y) \equiv \frac{\delta G^{\rm tr}_{mn}(x,x)}{\delta\varphi_l(y)}, \tag{A16}$$

and in the end we shall take $J_i(x) = 0$. It is obvious that at homogeneous condition, (A15) is equivalent to (18) developed with the Φ-derivable approach.

2. Detailed calculations

To get the corrections of the MHFB, we must calculate $I_{mn,m'n'}(k) = -\frac{1}{V\beta}\sum_{\omega_{n1},k_1} G^{\rm tr}_{mn}(k_1+k)G^{\rm tr}_{m'n'}(k_1)$. This can be done by the standard method of the summation of Matsubara frequencies.

For example, $G^{\rm tr}$ can be written in the form

$$G^{\rm tr} = \frac{1}{(i\omega_n)^2 - \omega_k^2}\begin{pmatrix} \Sigma^{\rm tr}_{11} & i\omega_n - k^2 + \mu_R \\ -i\omega_n - k^2 + \mu_R & \Sigma^{\rm tr}_{11}\end{pmatrix}$$

and then

$$\begin{aligned}
I_{11;11}(\omega_n,k) &= -\frac{1}{V\beta}\sum_{\omega_{n1},k_1} G^{\rm tr}_{11}(k_1+k)G^{\rm tr}_{11}(k_1)\\
&= -\frac{1}{V\beta}\sum_{k',\omega'_n}\frac{\Sigma^{\rm tr}_{11}}{(i\omega_n + i\omega'_n)^2 - \omega^2_{k+k'}}\frac{\Sigma^{\rm tr}_{11}}{(i\omega'_n)^2 - \omega^2_{k'}}\\
&= \frac{\Sigma^{\rm tr2}_{11}}{4V}\sum_{k'}\frac{1}{\omega_{k'}\omega_{k+k'}}\left[\left(\frac{1}{i\omega_n - \omega_{k+k'} - \omega_{k'}} - \frac{1}{i\omega_n + \omega_{k+k'} + \omega_{k'}}\right)\right.\\
&\quad + \frac{1}{e^{\beta\omega_{k'}} - 1}\left(\frac{1}{i\omega_n + \omega_{k'} - \omega_{k+k'}} - \frac{1}{i\omega_n + \omega_{k'} + \omega_{k+k'}}\right)\\
&\quad \left. + \frac{1}{e^{\beta\omega_{k+k'}} - 1}\left(\frac{1}{i\omega_n + \omega_{k+k'} - \omega_{k'}} - \frac{1}{i\omega_n + \omega_{k'} + \omega_{k+k'}}\right)\right].
\end{aligned}$$

The other $I_{mn,m'n'}(k)$ can be calculated in a similar way. And the summation of ω'_n is crucial for analytical continuation.

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