Tan's contact as an indicator of completeness and self-consistency of a theory

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It is well known that Tan's contact could be calculated by using any of the following three methods: by the asymptotic behavior of momentum distribution, by Tan's adiabatic sweep theorem, or by the operator product expansion as an expectation value of the interaction term. We argue that if a theory describing a Bose (or Fermi) system with the only contact interaction is self-consistent, then it should lead to the same result in all three cases. As an example, we considered mean-field theory (MFT)-based approaches and established that among existing approximations of MFT, the Hartree-Fock-Bogoliubov (HFB) approach is the most self-consistent. Actually, HFB is able to describe existing experimental data on Tan's contact for dilute Bose gas but fails to predict its expected behavior at large gas parameters ($\gamma > 0.015$). So, for appropriate description of properties of a Bose gas even at zero temperature, this approximation needs to be expanded by taking into account fluctuations in higher order then the second one.

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I. INTRODUCTION

The experimental discovery of superfluidity of ^{4}He at very low temperatures and atmospheric pressure and realization of Bose-Einstein condensation (BEC) of alkali atoms [1] have impacted development of various theories describing thermodynamics of the system of ultracold atoms. Most of them are based on field theoretical approaches, developed before for high energy physics, and nicely reviewed by Andersen [2]. In accordance with the classification proposed by Proukakis and Jackson, existing theoretical formalisms may be classified, loosely speaking, into three classes of approaches, based on certain common conceptual notions shared between them [3]. Namely, mean-field theories (MFTs), number-conserving perturbative treatments, and stochastic approaches. Although there is no universally accepted optimal theory for description of ultracold Bose gases at low temperatures, a researcher may prefer one of those approaches depending on the nature of his main goal. For example, when the dynamics or the behavior of the system at a critical point is not the issue, then MFT seems to be optimal.

Mean-field approaches for ultracold gases rely on spontaneous symmetry breaking, which mathematically manifests itself by splitting the Bose field operator $\psi(\mathbf{r}, t)$ into a mean-field condensate contribution $\phi(\mathbf{r}, t)$ and an operator describing fluctuations (quantum, thermal) about this mean field. After such splitting, also called a Bogoliubov shift [4], the full system Hamiltonian breaks down into various contributions as $H = H_0 + H_1 + H_2 + H_3 + H_4$ based on the number of condensate and noncondensate factors contained in each of them. For example, H_0 has no operators, while H_4 includes fluctuation operators in fourth order. Further, various approaches within MFT arise depending on the way of taking into account those fluctuations, since even a simple $\lambda\phi^4$ model has no analytical complete solution. For example, for weakly interacting ultracold Bose gases, characterized by a small diluteness gas parameter γ, one limits oneself to the simple Bogoliubov or one-loop approximation, when only H_2 term is taken into account. All and all, in general, each approximation in the framework of MFT leads to a closed system of equations with respect to self-energy, condensed fraction, etc. Obviously, these equations should be solved self-consistently, which requires the self-consistency of a chosen approach or a theory as a whole by itself.

In the present paper, we propose that evaluation of Tan's contact of a system with contact s-wave interaction may serve as a checkpoint for the self-consistency of a model. As an example, we shall consider various approximations within MFT and check their self- consistency by evaluation of Tan's contact in different ways.

Nearly 15 years ago, Tan introduced [5–7] a quantity, C which is further referred in the literature as a Tan's contact. By using rigorous mathematical methods to study the system of fermions with contact interaction, Tan obtained exact universal relations, which include the contact. He proved that this quantity measures the density of pairs at short distances and determines the exact large momentum or high-frequency behavior of various physical observables. Further, Tan's ideas were developed in Refs. [8–13] and his relations have been rederived and extended by using alternative methods. Particularly, Combescot *et al.* [13] have shown that Tan's relations are valid not only for fermions but also for bosons. It is remarkable that Tan's relations, including C, hold for any state of the system, few-body or many-body, homogenous or in a trapping potential, superfluid or normal, zero or nonzero temperatures [8].

Summarizing, Tan's contact for Bosons with zero range interaction may be theoretically evaluated (or measured experimentally) by using any of following equations [14]:

1. By the asymptotic behavior of momentum distribution n_k,

$$C_n = \lim_{k\to\infty} k^4 n_k, \tag{1}$$

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where n_k is normalized to the total number of particles N, such that $\sum_k n_k = N$. So,[1] C has a dimensionality length^{-4}.

2. By Tan's adiabatic sweep theorem as

$$C_E = \frac{8\pi ma^2}{V}\left(\frac{\partial E}{\partial a}\right), \tag{2}$$

where E and V are the total energy and volume of the system, respectively, a is the s-wave scattering length and m is the mass of particle. This equation manifests the relation between macroscopic thermodynamical parameter E and microscopic parameter a. Consequently, the variation of the total energy can be written in the following general form [14,15]:

$$dE = TdS - PdV + \mu dN + HdM + \frac{CV}{8\pi ma^2}da. \tag{3}$$

In this sense, Tan's contact and the scattering length may be considered as conjugate parameters of a system, regardless, in the superfluid or normal phase.

3. By the operator product expansion as an expectation value of the interaction term as [8]

$$C_\psi = \frac{(mg)^2}{V}\int d\mathbf{r}\langle\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\psi(\mathbf{r})\rangle, \tag{4}$$

where $g = 4\pi a/m$ is the coupling constant of zero range interaction.

From Eqs. (1)–(4), it is seen that for the case of quantum particles with pointlike interactions, short-range correlations are embedded in Tan's contact, which is proportional to the probability that two particles approach each other very closely.

Obviously, regardless of the way of evaluation (or measuring) of Tan's contact by using any of three Eqs. (1), (2), or (4), one is supposed to obtain the same value, i.e.,

$$C = C_n = C_E = C_\psi. \tag{5}$$

This trivial statement gives us an opportunity to check self-consistency of an applied theory. In the first part of the present paper, we shall derive explicit expressions for C and revise various versions of MFT in this way. In the second part of the paper, we shall compare our results with existing experimental data on C and make an attempt to predict its behavior at large gas parameter.

Presently, Tan's contact has been experimentally studied not only for fermions [16,17] but also for bosons at ultracold temperatures [18–21]. Particularly, Tan's relations on tails of the momentum distribution and the tail of the transition rate have been tested experimentally by using short time probes of ultracold atoms. Moreover, C plays an important role in the radio frequency (rf) spectroscopy [8]. As expected, the values of Tan's contact, obtained from both kinds of measurements, ballistic and rf spectroscopy show a good agreement [17].

The present paper is organized as follows. In Sec. II, we derive explicit expressions for Tan's contact in various approaches of MFT; in Sec. III, we shall study self-consistency of each approach by numerical analysis and compare our theoretical predictions with experimental values of C. In the last section, we present our conclusions. The details of calculations and summary of working equations are presented in Appendices A and B, respectively.

[1]Here and below, we adopt $\hbar = 1$ and $k_B = 1$ for convenience.

II. TAN'S CONTACT FOR HOMOGENOUS BOSE GAS IN MFT

A grand canonical ensemble of Bose particles with a short range s-wave interaction is governed by the Euclidian action [2],

$$S[\psi,\psi^\dagger] = \int_0^\beta d\tau\int d\vec{r}\{\psi^\dagger(\tau,\vec{r})[\partial_\tau - \frac{\nabla^2}{2m} - \mu]\psi(\tau,\vec{r}) + \frac{g}{2}[\psi^\dagger(\tau,\vec{r})\psi(\tau,\vec{r})]^2\}, \tag{6}$$

where $\psi^+(\tau,\vec{r})$ is a complex field operator that creates a boson at the position $\vec{r}$, μ is the chemical potential, $\beta = 1/T$ the inverse of temperature T. This corresponds to the Hamiltonian:

$$H = \int d\vec{r}\left\{\psi^+\left[-\frac{\nabla^2}{2m} - \mu\right]\psi + \frac{g}{2}(\psi^+\psi)^2\right\}. \tag{7}$$

The quantities, required for evaluation of Tan's contact, can be obtained by using following expressions:

$$\rho_1 = \langle\tilde{\psi}^\dagger\tilde{\psi}\rangle = \frac{1}{V}\sum_k n_k,\ F = \Omega + \mu N,\ E = F + TS,$$
$$\Omega = -T\ln Z,\quad Z = \int \mathcal{D}\psi\mathcal{D}\psi^+\exp\{-S[\psi,\psi^\dagger]\},$$
$$\langle(\tilde{\psi}^\dagger\tilde{\psi})^2\rangle = {\rho_0}^2 + \rho_0\int d\mathbf{r}[3\langle\psi_1^2\rangle + \langle\psi_2^2\rangle] + \frac{1}{4}\int d\mathbf{r}[\langle\psi_1^4\rangle + 2\langle\psi_1^2\psi_2^2\rangle + \langle\psi_2^4\rangle], \tag{8}$$

where ρ_1 is the density of uncondensed atoms, Ω free energy, S is the entropy, ρ_0 is the condensed fraction introduced by the standard Bogoliubov shift,

$$\psi(\tau,\mathbf{r}) = \sqrt{\rho_0} + \tilde{\psi}(\tau,\mathbf{r}), \tag{9}$$

and ψ_1, ψ_2 are the components of fluctuation field defined as

$$\tilde{\psi} = \frac{1}{\sqrt{2}}(\psi_1 + i\psi_2),\quad \tilde{\psi}^\dagger = \frac{1}{\sqrt{2}}(\psi_1 - i\psi_2). \tag{10}$$

After the insertion of Eqs. (10) into (6), the total effective action is separated as follows:

$$\begin{aligned}
&S = S_0 + S_1 + S_2 + S_3 + S_4,\\
&S_0 = \textstyle\int_0^\beta d\tau\int d\mathbf{r}\{-\mu\rho_0 + \frac{g{\rho_0}^2}{2}\},\\
&S_1 = \textstyle\int_0^\beta d\tau\int d\mathbf{r}\{\sqrt{2\rho_0}(g\rho_0 - \mu)\psi_1\},\\
&S_2 = \textstyle\frac{1}{2}\int_0^\beta d\tau\int d\mathbf{r}\{(\partial_\tau - \frac{\nabla^2}{2m} - \mu + 3g\rho_0)\psi_1^2\\
&+ (\partial_\tau - \frac{\nabla^2}{2m} - \mu + g\rho_0)\psi_2^2\},\\
&S_3 = \textstyle\frac{g\sqrt{\rho_0}}{\sqrt{2}}\int_0^\beta d\tau\int d\mathbf{r}\psi_1[\psi_1^2 + \psi_2^2],\\
&S_4 = \textstyle\frac{g}{8}\int_0^\beta d\tau\int d\mathbf{r}\{\psi_1^4 + 2\psi_1^2\psi_2^2 + \psi_2^4\}.
\end{aligned} \tag{11}$$

Equations (6)–(11) are exact equations of MFT for a homogenous Bose gas and cannot be evaluated exactly. The problem is hidden in the evaluation of the path integrals over the fluctuating fields: It is well known that there is no handbook of path integrals, so one has to use an approximation. The only case when the path integral can be evaluated explicitly is the so-called Gaussian integral, based on the following formula [22][2]:

$$\int \mathcal{D}\psi_1\mathcal{D}\psi_2 e^{-\frac{1}{2}\int dxdx'\psi_a(x)G^{-1}_{ab}(x,x')\psi_b(x')}e^{\int dx j_a(x)\psi_a(x)} = (\sqrt{\mathrm{Det}G})\exp\left[\frac{1}{2}\int dxdx' j_a(x)\bar{G}_{ab}(x,x')j_b(x')\right], \quad (12)$$

where $x = (\tau, \mathbf{r})$, and $\bar{G}_{ab}(x,y) = [G_{ab}(x,y) + G_{ba}(y,x)]/2$ is usually interpreted as a Green's function.

A. Gaussian approximation

As a first approach, we limit ourselves to the case when in Eqs. (11) the terms S_3 and S_4 are neglected.[3] From the explicit expression for S_2 in (11), one obtains the propagator $G_{ab}(x,x') = (1/V\beta)\sum_{n,k} G_{ab}(\omega_n,\mathbf{k})\exp(i\omega_n(\tau-\tau') + i\mathbf{k}(\mathbf{r}-\mathbf{r}'))$, where in momentum space

$$G(\omega_n,\mathbf{k}) = \frac{1}{\omega_n^2 + E_k^2}\begin{pmatrix}\varepsilon_k + g\rho_0 - \mu & \omega_n \\ -\omega_n & \varepsilon_k + 3g\rho_0 - \mu\end{pmatrix}, \quad (13)$$

$(a, b = 1, 2)$, and $\omega_n = 2\pi nT$ is the Matsubara frequency, $E_k = \sqrt{\varepsilon_k + 3g\rho_0 - \mu}\sqrt{\varepsilon_k + g\rho_0 - \mu}$ is the quasiparticle (Bogolon) dispersion with $\varepsilon_k = \mathbf{k}^2/2m$. Now using Eqs. (8), (12), and (A10) leads to the following free energy at zero temperature:

$$\Omega(T=0) = -V\mu\rho_0 + \frac{Vg\rho_0{}^2}{2} + \frac{1}{2}\sum_k (E_k - \varepsilon_k). \quad (14)$$

In a stable equilibrium, this should be minimized with respect to ρ_0 to give

$$\frac{\partial\Omega}{\partial\rho_0} = -V\mu + Vg\rho_0 = 0, \qquad \mu = g\rho_0. \quad (15)$$

Now inserting this chemical potential into E_k one obtains a linear at low momentum dispersion,

$$E_k = \sqrt{\varepsilon_k}\sqrt{\varepsilon_k + 2g\rho_0} = ck + O(k^3), \quad (16)$$

with the sound velocity $c = \sqrt{g\rho_0/m}$.

For the condensate depletion ρ_1 at zero temperature it is easy to obtain following equation:

$$\rho_1(T=0) = \frac{1}{2V}\sum_k\left[\frac{\varepsilon_k + g\rho_0}{E_k} - 1\right] \equiv \frac{1}{V}\sum_k n_k, \quad (17)$$

where we used Eqs. (8) and (A10), and hence

$$C_n(\text{Gaussian}) = \lim_{k\to\infty} k^4 n_k = (gm\rho_0)^2 = (4\pi a\rho)^2 n_0^2 = C_{\text{class}} n_0^2, \quad (18)$$

where $n_0 = \rho_0/\rho$ is the condensate fraction, $\gamma = a^3\rho$ is the gas parameter, and $C_{\text{class}} = 16\pi^2\gamma^2/a^4$ is the Tan's contact, corresponding to the case when all fluctuations have been neglected. When the total number of particles (not the chemical potential) is fixed and given by the density ρ, the density of condensate ρ_0 in the above equations can be found as a solution to the following equation:

$$\rho_0 = \rho - \rho_1 = \rho - \frac{1}{2V}\sum_k\left[\frac{\varepsilon_k + g\rho_0}{\sqrt{\varepsilon_k}\sqrt{\varepsilon_k + 2g\rho_0}} - 1\right] = \rho - \frac{(mg\rho_0)^{3/2}}{3\pi^2}. \quad (19)$$

Now we pass to calculation of C_E, defined by (2). First, using Eqs. (14) and (15), we represent the total energy at zero temperature as

$$E = \Omega + \mu N = \frac{Vg\rho^2}{2} - \frac{Vg\rho_1^2}{2} + \frac{1}{2}\sum_k (E_k - \varepsilon_k). \quad (20)$$

Following the ideology of the Gaussian approach, when the fluctuations, explicitly higher than first order, are neglected, we can rewrite the last equation as

$$E = E_0 + E_{\text{fluc}}, \quad E_0 = \frac{Vg\rho^2}{2},$$
$$E_{\text{fluc}} = \frac{V}{4\pi^2}\int_0^\infty k^2 dk(\sqrt{\varepsilon_k}\sqrt{\varepsilon_k + 2g\rho_0} - \varepsilon_k). \quad (21)$$

The integral in Eqs. (21) is divergent. This may be evaluated by using dimensional regularization [23] or just by subtracting infinite parts from the integrand, leading to the same result. So, using the method of subtraction, one may easily obtain

$$E_{\text{fluc}} = \frac{1}{2}\sum_k (E_k - \varepsilon_k) \to \frac{1}{2}\sum_k\left[E_k - \varepsilon_k - g\rho_0 + \frac{(g\rho_0)^2}{2\varepsilon_k}\right] = \frac{8Vm^{3/2}(g\rho_0)^{5/2}}{15\pi^2}. \quad (22)$$

Taking the derivative with respect to a requires an explicit expression for $d\rho_0/da$, which could be obtained by differentiation of both sides of (19) and solving it with respect to $d\rho_0/da$. This gives

$$\frac{d\rho_0}{da} = -\frac{\rho_0}{a}\frac{1}{(1 + \frac{\sqrt{\pi}}{4\sqrt{n_0\gamma}})}. \quad (23)$$

Finally, by using Eqs. (2), (22), and (23), we obtain

$$C_E(\text{Gauss}) = C_{\text{class}}\left[1 + \frac{64 n_0^{5/2}\sqrt{\gamma}}{3(\sqrt{\pi} + 4\sqrt{\gamma n_0})}\right]. \quad (24)$$

As to the C_ψ, defined by (4), it can be easily found from Eqs. (8) and (A10) as

$$C_\psi = C_{\text{class}}[1 + 2(n_1 + \tilde{\sigma})], \quad (25)$$

[2]Here, there is a summation over repeated indices $(a, b = 1, 2)$.

[3]In quantum field theory, this corresponds to the one-loop approximation.

where $n_1 = \rho_1/\rho$. In Eq. (25), we neglected higher order fluctuations and introduced the fraction of anomalous density as $\tilde{\sigma} = (\langle \tilde{\psi}^+ \tilde{\psi}^+ + \tilde{\psi}\tilde{\psi} \rangle)/2\rho$.

B. Optimized Gaussian approximation

In the previous subsection, we have taken into account the depletion ρ_1 and anomalous density σ only up to the linear order, neglecting the terms S_3 and S_4 in Eqs. (11). Below we extend those relations for Tan's contact by taking into account quantum fluctuations in a more accurate way. For this purpose, we employ variational perturbation theory, developed by Stevenson many years ago [24] for the $\lambda\phi^4$ theory and further referred to as a δ-expansion method [25]. In this method, one introduces an auxiliary parameter δ and uses a perturbative scheme in a power series of δ, which is set to unity at the end of calculations. Note that the main disadvantage of this theory is that there is an arbitrariness in the choice of the expansion parameter δ.

For the effective action (6), the method includes two variational parameters, which may be fixed by principle of minimal sensitivity. In the present section, we apply variational perturbation theory to derive explicit expressions for Tan's contact , limiting ourselves to the first order in δ, which is referred to in the literature as an optimized Gaussian approximation. This will give us an opportunity to take into account ρ_1 as well as σ up to second order explicitly. Below we present the main equations needed for calculation of Tan's contact, referring the reader to the Appendix A for details. Note that the present approximation is equivalent to the Hartree-Fock-Bogoliubov (HFB) approach [3,4] used in Hamiltonian formalism. The preference of the path integral formalism is that, in contrast to Hamiltonian one, it gives a natural opportunity for going beyond HFB approximation, as was shown by Stancu and Stevenson [26].

Thus, for the free energy and densities, we have[4]

$$\begin{aligned}\Omega(T=0) &= -N\mu + \frac{Vg\rho^2}{2} + \frac{Vg({\rho_1}^2 - 2\rho_1\sigma - \sigma^2)}{2} \\ &\quad + \frac{1}{2}\sum_k (E_k - \varepsilon_k), \\ \rho_1(T=0) &= \frac{1}{2V}\sum_k \left[\frac{\varepsilon_k + \Delta}{E_k} - 1\right] \equiv \frac{1}{V}\sum_k n_k \\ &= \frac{(\Delta m)^{3/2}}{3\pi^2}, \\ \sigma(T=0) \equiv \rho\tilde{\sigma} &= -\frac{\Delta}{2V}\sum_k \left[\frac{1}{E_k} - \frac{1}{\varepsilon_k}\right] \\ &= \frac{(\Delta m)^{3/2}}{\pi^2} \approx \frac{\Delta m^{3/2}}{\pi^2}\sqrt{g\rho_0},\end{aligned} \tag{26}$$

where the energy dispersion is similar to the Bogoliubov one:

$$E_k = \sqrt{\varepsilon_k}\sqrt{\varepsilon_k + 2\Delta}. \tag{27}$$

For the zero-temperature energy, from the relation $E = \Omega + V\rho\mu$, one obtains

$$\begin{aligned}E(T=0) &= \frac{Vg\rho^2}{2} + \frac{Vg}{2}[{\rho_1}^2 - \sigma^2 - 2\rho_1\sigma] \\ &\quad + \frac{1}{2}\sum_k \left(E_k - \varepsilon_k - \Delta + \frac{\Delta^2}{2\varepsilon_k}\right) \\ &= \frac{Vg\rho^2}{2} + \frac{Vg}{2}[{\rho_1}^2 - \sigma^2 - 2\rho_1\sigma] + \frac{8V\Delta^{5/2}m^{3/2}}{15\pi^2},\end{aligned} \tag{28}$$

where the subtraction terms were introduced. Equations (26)–(28) include a key parameter Δ, which may be found by the physical solution ($\Delta \geqslant 0$) of the following equation of MFT:

$$\Delta = g(\rho_0 + \sigma) = g(\rho - \rho_1 + \sigma). \tag{29}$$

This equation gives the following explicit expression for the derivative of Δ with respect to a as

$$\Delta'_a = \frac{\Delta}{a}\frac{1}{[1 + 6\pi a(\rho_1 - \sigma)/m\Delta]}, \tag{30}$$

which is needed for evaluation of dE/da by using Eqs. (2) and (28). Therefore, in the HFB approach, we obtain the following expressions for Tan's contact:

$$C_n = (\Delta m)^2 = (cm)^4, \tag{31}$$

$$\begin{aligned}C_E &= C_{\text{class}}(1 + W_E), \\ W_E &= n_\sigma + \Delta'_a\left[\tfrac{2mn_1}{\pi\rho} + \tfrac{3an_\sigma}{\Delta}\right],\end{aligned} \tag{32}$$

$$\begin{aligned}C_\psi &= C_{\text{class}}(1 + W_\psi), \\ W_\psi &= 2(n_1 + \tilde{\sigma} - 2n_1\tilde{\sigma}) - n_\sigma,\end{aligned} \tag{33}$$

with $n_\sigma = n_1^2 - \tilde{\sigma}^2 - 2n_1\tilde{\sigma}$. From Eq. (31), it is seen that Tan's contact C_n, calculated from the tail of density distribution, is related to the sound velocity $c = \sqrt{\Delta/m}$ and may be directly observed experimentally by sound velocity measurements.

C. Bogoliubov approach

In the Bogoliubov approximation [27], the energy dispersion and the total energy are given as

$$\begin{aligned}E_k &= \sqrt{\varepsilon_k}\sqrt{\varepsilon_k + 2g\rho}, \\ E(T=0) &= \frac{Vg\rho^2}{2} + \frac{1}{2}\sum_k \left(E_k - \varepsilon_k - g\rho + \frac{(g\rho)^2}{2\varepsilon_k}\right) \\ &= \mu\frac{2V\pi\gamma^2}{ma^5}\left[1 + \frac{128\sqrt{\gamma}}{15\sqrt{\pi}}\right],\end{aligned} \tag{34}$$

and hence

$$C_E = C_{\text{class}}\left[1 + \frac{64\sqrt{\gamma}}{3\sqrt{\pi}}\right]. \tag{35}$$

Remarkably, the expression for the total energy in (34) coincides with one obtained many years ago by Lee, Huang, and Yang (LHY) [28] in a hard-core boson model, and Eq. (35) for C_E with the result by Schakel [29] derived in a similar way.

[4]See Appendix A for details.

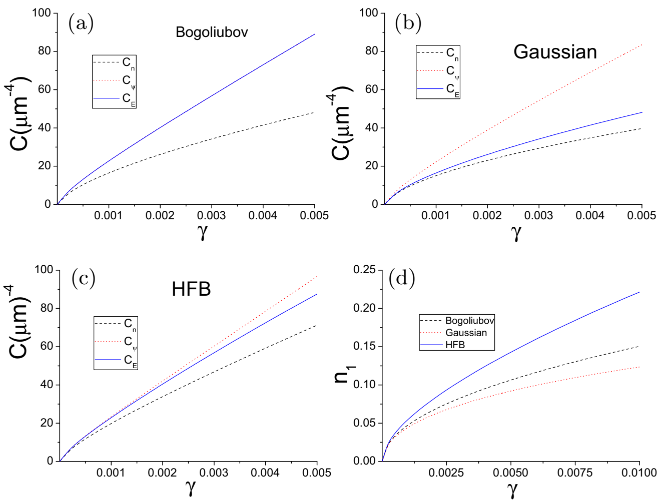

FIG. 1. Tan's contact as a function of the gas parameter $\gamma = \rho a^3$ in Bogoliubov (a), Gaussian (b), and HFB approximations (c). Dashed, solid, and dotted lines are obtained with Eqs. (1), (2) and (4), respectively. The corresponding condensate depletions, $n_1 = N_1/N$, are presented in Fig. 1(d).

A question arises: What is the difference between Gaussian and Bogoliubov approximations? The main difference is that in Gaussian approximation, one has to preliminary solve Eq. (19) with respect to ρ_0 for a given γ, while in Bogoliubov, there is no need to solve any equation. This fact makes the Bogoliubov approximation attractive and the most practical one to make a fast estimation of a physical quantity in the BEC regime.

Formally, Eqs. (34) may be derived from the HFB approach by setting $\Delta = g\rho$, ${\rho_1}^2 \to 0$ and $\sigma \to 0$ explicitly in Eqs. (26)–(28). So, particularly, one obtains

$$\rho_1(T=0) = \frac{1}{2V}\sum_k\left[\frac{\varepsilon_k + g\rho}{\sqrt{\varepsilon_k}\sqrt{\varepsilon_k + 2g\rho}} - 1\right]$$
$$\equiv \frac{1}{V}\sum_k n_k = \frac{(g\rho m)^{3/2}}{3\pi^2},$$
$$n_0 = 1 - \frac{\rho_1}{\rho} = 1 - \frac{8\sqrt{\gamma}}{3\sqrt{\pi}},$$
$$C_n = C_\psi = C_{\text{class}}. \quad (36)$$

From Eqs. (36), one may conclude that the Bogoliubov approximation takes into account the gas parameter up to first order in the expansion by $\sqrt{\gamma}$ in evaluation of the condensed fraction. The net results of the present section are summarized in Table I of Appendix B.

III. RESULTS AND DISCUSSIONS

Now we are in the position of studying three versions of MFT for self-consistency in the spirit of the requirement in Eq. (5). In Fig. 1, we present Tan's contact obtained in Bogoliubov [Fig. 1(a)], Gaussian [Fig. 1(b)], and HFB [Fig. 1(c)] approximations. Here dashed, solid, and dotted curves correspond to C_n, C_E, and C_ψ defined by Eqs. (1), (2), and (4), respectively. From Fig. 1(a), it is seen that the Bogoliubov approximation satisfies the first equality $C_n = C_\psi$, but not the second one, i.e., $C_\psi \neq C_E$. As to the Gaussian (one-loop) approximation, the difference between these three quantities is rather notable [see Fig. 1(b)]. In this sense, the Bogoliubov approximation seems more reliable than the Gaussian one. This fact can explain popularity of Bogoliubov approximation, including LHY terms [28] in the literature [18,30]. From Fig. 1(c), it is seen that the discrepancy between C_n, C_E, and C_ψ is rather small for the variational Gaussian approximation. Hence, one may conclude that the HFB approximation can be regarded as the most complete and self-consistent one among other existing MFT-based approaches. Nevertheless, strongly speaking, HFB is also needed for corrections, especially for $\gamma > 0.002$, arising from the higher order quantum fluctuations. The intensity of such fluctuations is almost proportional to the fraction of uncondensed particles n_1. As seen from Fig. 1(d), even at $\gamma \sim 0.005$ the depletion is about 15%. Note that, in superfluid helium ^{4}He, $n_1 \approx 90\%$.

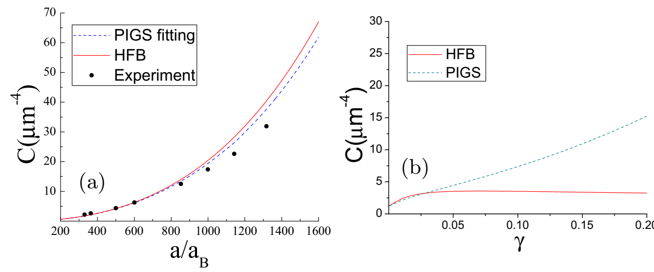

FIG. 2. (a) The contact in natural units $(\mu\text{m})^{-4}$ versus scattering length a computed in PIGS Monte Carlo method [31] (dashed curve) and HFB approaximation (solid curve). Filled circles are experimental data of Wild *et al.* [18] obtained for ^{85}Rb atomic condensate. The scattering length a is given in units of the Bohr radius $a_B = 5.310^{-5}\mu$m, (b) Tan's contact at large values of the gas parameter ρa^3 in HFB (solid line), and PIGS Monte Carlo (dashed line) [31]. In both panels, the density is fixed in its typical value as $\rho = 5.8\mu\text{m}^{-3}$.

On the other hand, one may judge about an appropriateness of any theory just by comparing its predictions with experimental measurements. In Fig. 2(a), we compare our predictions for Tan's contact given by the HFB approach with the experimental data on ^{85}Rb atomic condensate at fixed density $\rho = 5.8\,\mu\text{m}^{-3}$. It is seen that the HFB approximation is able to describe C rather satisfactorily up to $a/a_B < 1200$, which corresponds to $\gamma \approx 0.0015$. Moreover, HFB predictions for the Tan's contact is in a good agreement with path-integral ground-state (PIGS) Monte Carlo calculations performed by Rossi and Salasnich [31].

Unfortunately, presently, Tan's contact for a Bose gas has been measured at very small values of the gas parameter, $\gamma \leqslant 0.002$. To predict its behavior at larger γ, we calculated Tan's contact in the region $0 \leqslant \gamma \leqslant 0.2$[5] and presented the results in Fig. 2(b). It is seen that the PIGS Monte Carlo method predicts a smooth increasing of C, while the latter remains practically unchanged in the HFB approximation for $\gamma > 0.05$.

[5]For superfluid helium, $\gamma \approx 0.6$

IV. CONCLUSION

We have derived explicit expressions for Tan's contact of bosons at zero temperature within various approximations based on MFT. Numerical analysis made with these equations gave us an opportunity to study such approximations for completeness and self-consistency. We have shown that in this concept, the HFB approximation, derived within optimized Gaussian perturbation theory, satisfies the requirement $C_n = C_E = C_\psi$ better than one-loop or Bogoliubov approximations.

Moreover, HFB predictions are in a good agreement with existing experimental data as well as with Monte Carlo calculations for small values of the gas parameter. However, for large values of γ, HFB needs serious corrections. These could be performed by an extension of the present approach in the spirit of post-Gaussian perturbative approximation, which includes the second-order δ expansion [26]. It is expected that such an extension could give rise to a desired logarithmic term, which is used in the literature [29,31,32]. The work is in progress.

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APPENDIX A: DERIVATION OF Ω

In this Appendix, we present the derivation of the free energy Ω given in Eqs. (26). Inserting Eq. (9) into the action Eq. (6), the latter can be divided into the following parts:

$$
\begin{aligned}
S &= S_0 + S_1 + S_2 + S_3 + S_4,\\
S_0 &= \int_0^\beta d\tau \int d\vec{r}\left\{-\mu\rho_0 + \frac{g\rho_0^2}{2}\right\},\\
S_1 &= \int_0^\beta d\tau \int d\vec{r}\{[g\rho_0^{3/2} - \mu\sqrt{\rho_0}]\tilde{\psi} + \text{H.c.}\},\\
S_2 &= \int_0^\beta d\tau \int d\vec{r}\left\{\tilde{\psi}^\dagger\left(\partial_\tau - \frac{\nabla^2}{2m} + 2g\rho_0 - \mu\right)\tilde{\psi} + \frac{g\rho_0}{2}(\tilde{\psi}^{\dagger 2} + \tilde{\psi}^2)\right\},\\
S_3 &= g\sqrt{\rho_0}\int_0^\beta d\tau \int d\vec{r}\{\tilde{\psi}^\dagger\tilde{\psi}^2 + \tilde{\psi}^{\dagger 2}\tilde{\psi}\},\\
S_4 &= \frac{g}{2}\int_0^\beta d\tau \int d\vec{r}\tilde{\psi}^\dagger\tilde{\psi}^\dagger\tilde{\psi}\tilde{\psi}.
\end{aligned}
\tag{A1}
$$

Now employing the δ-expansion method, we add to the total action Eqs. (A1) the term $(1-\delta)\int_0^\beta d\tau\int d\vec{r}[\Sigma_n(\tilde{\psi}^\dagger\tilde{\psi}) + (1/2)\Sigma_{an}(\tilde{\psi}^\dagger\tilde{\psi}^\dagger + \tilde{\psi}\tilde{\psi})]$ and make replacement $g \to \delta g$. Then, after presenting $\tilde{\psi}$ and $\tilde{\psi}^+$ in Cartesian form as

$$
\begin{aligned}
\tilde{\psi} &= \frac{1}{\sqrt{2}}(\psi_1 + i\psi_2),\\
\tilde{\psi}^\dagger &= \frac{1}{\sqrt{2}}(\psi_1 - i\psi_2),
\end{aligned}
\tag{A2}
$$

the total action may be rewritten as follows [33]:

$$
\begin{aligned}
S &= S_0 + S_{\text{free}} + S_{\text{int}},\\
S_{\text{free}} &= \frac{1}{2}\int_0^\beta d\tau \int d\vec{r}\left\{i\epsilon_{ab}\psi_a\partial_\tau\psi_b + \psi_1\left(-\frac{\nabla^2}{2m} + X_1\right)\psi_1 + \psi_2\left(-\frac{\nabla^2}{2m} + X_2\right)\psi_2\right\},\\
S_{\text{int}} &= S_{\text{int}}^{(1)} + S_{\text{int}}^{(2)} + S_{\text{int}}^{(3)} + S_{\text{int}}^{(4)},\\
S_{\text{int}}^{(1)} &= \delta\int_0^\beta d\tau \int d\vec{r}\{\psi_1\sqrt{2}\rho_0(-\mu + g\rho_0)\},\\
S_{\text{int}}^{(2)} &= \frac{\delta}{2}\int_0^\beta d\tau \int d\vec{r}\{\beta_1\psi_1^2 + \beta_2\psi_2^2\},\\
S_{\text{int}}^{(3)} &= \frac{\delta g\sqrt{2}\rho_0}{2}\int_0^\beta d\tau \int d\vec{r}\{(\psi_1^2 + \psi_2^2)\psi_1\},\\
S_{\text{int}}^{(4)} &= \frac{\delta g}{8}\int_0^\beta d\tau \int d\vec{r}\{\psi_1^4 + 2\psi_1^2\psi_2^2 + \psi_2^4\},
\end{aligned}
\tag{A3}
$$

where

$$
\beta_1 = -\mu - X_1 + 3g\rho_0, \quad \beta_2 = -\mu - X_2 + g\rho_0, \tag{A4}
$$

and X_1 and X_2 are the variational parameters, related to the normal Σ_n and anomalous Σ_{an} self-energies as $X_1 = \Sigma_n + \Sigma_{\text{an}} - \mu$ and $X_2 = \Sigma_n - \Sigma_{\text{an}} - \mu$. The free energy Ω can be evaluated as

$$
\Omega = -T\ln Z(j_1, j_2)|_{j_1=0, j_2=0}, \tag{A5}
$$

where the grand partition function is

$$
\begin{aligned}
Z(j_1, j_2) &= e^{-S_0}\int D\psi_1 D\psi_2 e^{-\frac{1}{2}\int dx\int dx'\psi_a(x)G_{ab}^{-1}(x,x')\psi_b(x')}\\
&\quad\times e^{-S_{\text{int}}}e^{\int dx[j_1(x)\psi_1(x) + j_2(x)\psi_2(x)]},
\end{aligned}
\tag{A6}
$$

in which we introduced $x = (\tau, \vec{r})$ and $\int dx \equiv \int_0^\beta d\tau\int d\vec{r}$. For a uniform system, the Green's function is translationally invariant,

$$
G_{ab}(\vec{r}, \tau; \vec{r}', \tau') = \frac{1}{V\beta}\sum_{n,k} e^{i\omega_n(\tau-\tau')}e^{i\vec{k}(\vec{r}-\vec{r}')}G_{ab}(\vec{k}, \omega_n), \tag{A7}
$$

with

$$
\begin{aligned}
G_{11}(\vec{k}, \omega_n) &= \frac{\epsilon_k + X_2}{\omega_n^2 + E_k^2},\\
G_{22}(\vec{k}, \omega_n) &= \frac{\epsilon_k + X_1}{\omega_n^2 + E_k^2},\\
G_{12}(\vec{k}, \omega_n) &= \frac{\omega_n}{\omega_n^2 + E_k^2},\\
G_{21}(\vec{k}, \omega_n) &= -G_{12}(\vec{k}, \omega_n),\\
E_k^2 &= (\epsilon_k + X_1)(\epsilon_k + X_2),
\end{aligned}
\tag{A8}
$$

where $\omega_n = 2\pi nT$ is the Matsubara frequency. In the path integral formalism, the expectation value of an operator

$\langle\hat{O}(\tilde{\psi}^{+},\tilde{\psi})\rangle$ is defined as

$$\langle\hat{O}\rangle=\frac{1}{Z_0}\int D\tilde{\psi}^{\dagger}D\tilde{\psi}\hat{O}(\tilde{\psi}^{\dagger},\tilde{\psi})e^{-S(\tilde{\psi}^{\dagger},\tilde{\psi})}, \quad (A9)$$

where $Z_0=Z(j_1=0,j_2=0,S_{\rm int}=0)$ is the noninteracting partition function.

Particularly, using the well-known formula (12) and following identities:

$$\begin{aligned}\ln{\rm Det}[G^{-1}]&=\sum_{n,k}\ln(E_k^2+\omega_n^2)\\&=\sum_k[\beta E_k+2\ln(1-e^{-\beta E_k})],\\&\times\sum_{n=-\infty}^{n=\infty}\frac{1}{(\omega_n^2+E_k^2)}=\frac{\beta}{2E_k}\coth(\beta E_k/2),\end{aligned} \quad (A10)$$

one may show that [34]

$$\begin{aligned}&\langle\hat{O}(\psi_a(x)\psi_b(y))\rangle=\hat{O}\big(\tfrac{\delta}{\delta j_a(x)},\tfrac{\delta}{\delta j_b(y)}\big)\\&\exp\big[\tfrac{1}{2}\textstyle\int j_a(x)G_{ab}(x,y)j_b(y)dxdy\big],\\&\langle\psi_a(x)\rangle=0,\quad\langle\psi_a(x)\psi_b(x')\rangle=G_{ab}(x,x'),\\&\langle\psi_1(x)\psi_2(x)\rangle=G_{12}(0)\\&=\tfrac{1}{V\beta}\textstyle\sum_n G_{12}(\vec{k},\omega_n)=\tfrac{1}{V\beta}\sum_{n=-\infty}^{\infty}\tfrac{\omega_n}{\omega_n^2+E_k^2}=0,\\&\langle\psi_a^4(x)\rangle=3G_{aa}^2(0),\\&\langle\psi_1^2(x)\psi_2^2(x)\rangle=G_{11}(0)G_{22}(0),\\&G_{ab}(0)\equiv\tfrac{1}{V\beta}\textstyle\sum_{k,n}G_{ab}(k,\omega_n),\\&\langle\psi_{a_1},\psi_{a_2}\dots\psi_{a_n}\rangle=0,\quad n=1,3,5\dots.\end{aligned} \quad (A11)$$

We now expand $\exp(-S_{\rm int})$ in Eqs. (A3) in powers of δ:

$$e^{-S_{\rm int}}=1-S_{\rm int}^{(1)}-S_{\rm int}^{(2)}-S_{\rm int}^{(3)}-S_{\rm int}^{(4)}+O(\delta^2). \quad (A12)$$

Expressing the "noninteracting" partition function as

$$\begin{aligned}Z_0(j)&=\int D\psi_1D\psi_2e^{-\frac{1}{2}\int dxdx'\psi_a(x)G_{ab}^{-1}(x,x')\psi_b(x')}e^{\int dx j_a(x)\psi_a(x)}\\&=(\sqrt{{\rm Det}G})\exp\left[\frac{1}{2}\int dxdx'j_a(x)\bar{G}_{ab}(x,x')j_b(x')\right],\end{aligned} \quad (A13)$$

where $\bar{G}_{ab}(x,y)=[G_{ab}(x,y)+G_{ba}(y,x)]/2$, one may obtain

$$Z(j)=e^{-S_0}\big[Z_0(j)-\langle S_{\rm int}^{(1)}\rangle-\langle S_{\rm int}^{(2)}\rangle-\langle S_{\rm int}^{(3)}\rangle-\langle S_{\rm int}^{(4)}\rangle\big], \quad (A14)$$

where $\langle\hat{O}\rangle=[\int D\psi_1D\psi_2e^{-S_{\rm free}}\hat{O}(\psi_1,\psi_2)]/Z_0(j)|_{(j=0)}$ and $Z_0(j)|_{(j=0)}=1/\sqrt{{\rm Det}\,G^{-1}}$. The expectation values in (A14) can be easily calculated by using Eqs. (A11) as

$$\begin{aligned}&\langle S_{\rm int}^{(1)}\rangle=0,\quad\langle S_{\rm int}^{(3)}\rangle=0,\\&\langle S_{\rm int}^{(2)}\rangle=\tfrac{1}{2}\textstyle\int dx(\beta_1G_{11}(0)+\beta_2G_{22}(0))=\tfrac{\beta}{2}(\beta_1B+\beta_2A),\\&\langle S_{\rm int}^{(4)}\rangle=\tfrac{g\beta}{8}[3G_{11}^2(0)+3G_{22}^2(0)+2G_{11}(0)G_{22}(0)]\\&=\tfrac{g\beta}{8}[3B^2+3A^2+2AB],\end{aligned} \quad (A15)$$

where $A=V(\rho_1-\sigma)$, $B=V(\rho_1+\sigma)$. Thus, using the formula $\ln(1+x)\approx x$, we obtain

$$\Omega=-T\ln Z(j)|_{j=0}=TS_0-T\ln Z_0+T\langle S_{\rm int}^{(2)}\rangle+T\langle S_{\rm int}^{(4)}\rangle, \quad (A16)$$

where we set $\delta=1$. Finally, using (A15) gives

$$\begin{aligned}&\Omega=\Omega_0+\Omega_{\rm free}+\Omega_2+\Omega_4,\\&\Omega_0=-\mu V\rho_0+\tfrac{gV\rho_0{}^2}{2},\\&\Omega_{\rm free}=\tfrac{1}{2}\textstyle\sum_k(E_k-\epsilon_k)+T\sum_k\ln(1-e^{-\beta E_k}),\\&\Omega_2=\tfrac{1}{2}[\beta_1B+\beta_2A],\\&\Omega_4=\tfrac{g}{8V}[3A^2+3B^2+2AB],\end{aligned} \quad (A17)$$

In the above equations, $X_1\equiv2\Delta$ can be found from equation $\partial\Omega/\partial X_1=0$ which leads to MFA Eq. (29). As to X_2 it should be set to zero, $X_2=0$, to make the dispersion similar to the Bogoliubov one: $E_k=\sqrt{\varepsilon_k}\sqrt{\varepsilon_k+2\Delta}$ in accordance with Hugenholtz-Pines theorem [35]. As a result, one obtains

$$\begin{aligned}&X_1=2g(\rho_0+\sigma)=2g\rho+2g(\sigma-\rho_1),\\&\mu=g\rho+g\rho_1-g\sigma.\end{aligned} \quad (A18)$$

APPENDIX B: SUMMARY OF MAIN EQUATIONS IN VARIOUS APPROACHES OF MFT

We present the total energy of a Bose system at $T=0$ as

$$E=\frac{V\rho^2g}{2}(1+\tilde{E}_0)+\frac{8Vm^{3/2}}{15\pi^2}\tilde{E}_{\rm fluc}, \quad (B1)$$

where $\tilde{E}_0$ and $\tilde{E}_{\rm fluc}$ are shown on Table I (columns IV and V). Tan's contact, calculated from any of Eqs. (1)–(4), may be simply presented as $C_x=16\pi^2a^2\rho^2(1+W_x)$, $(x=n,E,\psi)$ where W_x are given in columns VI–VIII of Table I. The second column of this table includes equations for the condensed fraction ρ_0 and for the reduced self-energy $\Delta=(\Sigma_n+\Sigma_{\rm an}-\mu)/2$. Note that ρ_0 is fixed as $\rho_0=n_0\rho=\rho(1-8\sqrt{\gamma}/3\sqrt{\pi})$ in the Bogoliubov approximation, while it should be numerically evaluated as solutions of MFT equations in other approaches.

TABLE I. MFT equations, the total energy, and Tan's contact in MFT.

MFT app.	ρ_0 and MFT equations	Dispersion	$\tilde{E}_0$	$\tilde{E}_{\text{fluc}}$	W_n	W_E	W_ψ
HFB	$\rho_0 = \rho - \rho_1$ $\Delta = g(\rho_0 + \sigma)$ $\rho_1 = (\Delta m)^{3/2}/3\pi^2$ $\sigma = m^{3/2}\Delta\sqrt{g\rho_0}/\pi^2$	$E_k = \sqrt{\varepsilon_k}\sqrt{\varepsilon_k + 2\Delta}$	$\tilde{E}_0 = n_1^2 - \tilde{\sigma}^2 - 2n_1\tilde{\sigma}$	$\Delta^{5/2}$	$(n_1 - \tilde{\sigma})*$ $(n_1 - \tilde{\sigma} - 2)$	$n_\sigma + \Delta'_a[\frac{2mn_1}{\pi\rho} + \frac{3an_\sigma}{\Delta}]$ $n_\sigma = n_1^2 - \tilde{\sigma}^2 - 2n_1\tilde{\sigma}$ $\Delta'_a = \frac{\Delta}{a}\frac{1}{[1+6\pi a(\rho_1-\sigma)/m\Delta]}$	$2(n_1 + \tilde{\sigma} -$ $2n_1\tilde{\sigma}) - n_\sigma$
Gaussian	$\tilde{n}_0{}^3 + p\tilde{n}_0{}^2 - p = 0,$ $\tilde{n}_0 = \sqrt{n_0},$ $p = 3\sqrt{\pi}/8\sqrt{\gamma}$	$E_k = \sqrt{\varepsilon_k}\sqrt{\varepsilon_k + 2g\rho_0}$	0	$(g\rho_0)^{5/2}$	$n_1(n_1 - 2)$	$\frac{64n_0^{5/2}\sqrt{\gamma}}{3(\sqrt{\pi}+4\sqrt{\gamma n_0})}$	$\frac{64n_0^{3/2}\sqrt{\gamma}}{3\sqrt{\pi}}$
Bogoliubov	$n_0 = 1 - 8\sqrt{\gamma}/3\sqrt{\pi}$	$E_k = \sqrt{\varepsilon_k}\sqrt{\varepsilon_k + 2g\rho}$	0	$(g\rho)^{5/2}$	1	$\frac{64\sqrt{\gamma}}{3\sqrt{\pi}}$	$\frac{64\sqrt{\gamma}}{3\sqrt{\pi}}$

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