Non-perturbative Predictions for Cold Atom Bose Gases with Tunable Interactions

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Abstract

We derive a theoretical description for dilute Bose gases as a loop expansion in terms of composite-field propagators by rewriting the Lagrangian in terms of auxiliary fields related to the normal and anomalous densities. We demonstrate that already in leading order this non-perturbative approach describes a large interval of coupling-constant values, satisfies Goldstone's theorem, yields a Bose-Einstein transition that is second-order, and is consistent with the critical temperature predicted in the weak-coupling limit by the next-to-leading order large-N expansion.

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Nearly a century after the first observation of the lambda transition in liquid helium[1], a quantitative, first-principles description of strongly-correlated bosons remains a challenge. After the transition was recognized as the onset of superfluidity[2], the connection with Bose-Einstein condensation (BEC) was proposed[3], but it was Bogoliubov's work[4] pointing out that the dispersion of the elementary BEC excitations satisfy the Landau criterion for superfluidity[5] that motivated weakly-interacting BEC studies to investigate superfluid properties. In weakly-interacting systems, the many-body properties do not depend on the shape of the interaction potential, but only on the s-wave scattering length, a_0, and the boson fluid acts as point-like interacting particles[6].

Unlike liquid helium, cold atoms remain point-like even when the scattering length is tuned near a Feshbach resonance. Then, strongly-correlated cold atom bosons offer the exciting prospect of studying point-like strongly interacting bosons, possibly in the universal regime where the scattering length greatly exceeds the inter-particle distance and the latter becomes the only relevant length scale[7]. This hope appeared thwarted when it was shown that the three-body loss rate in cold atom traps scales as a_0^4 near a Feshbach resonance[8]. In accordance, the universal regime was reached only in ultra-cold fermionic gases[9], where the three-body loss is reduced by virtue of the Pauli exclusion principle. However, the recent observation that three-body losses are strongly suppressed in optical lattices when the average number of bosons per site is two or less[10], rekindles the prospect of studying medium and strongly-correlated cold atom bosons. Novel cold-atom trap technologies that produce stable, flat potentials bound by a sharp edge[11], suggest the study of finite-temperature properties such as the BEC transition temperature T_c and the superfluid to normal fluid ratio and depletion, at fixed density, ρ.

At finite temperature, the description of BEC's remains a challenge even in the weakly-interacting regime. Standard approximations such as the Hartree-Fock-Bogoliubov and the Popov schemes, generally fall within the Hohenberg and Martin classification[12] of conserving and gapless approximations, which implies that they either violate Goldstone's theorem or general conservation laws[13]. These approximations generally predict the BEC transition to be a first-order transition, whereas we expect the transition to be second order[14].

In this paper, we present a new theoretical framework that describes a large interval of $\rho^{1/3}a_0$-values, satisfies Goldstone's theorem and yields a Bose-Einstein transition that is second-order, while also predicting reasonable values for the depletion. Furthermore, this framework can predict *all* experimentally relevant quantities within the same calculation, determining fully consistently quantities such as T_c, the collective mode frequencies[15] and the compressibility (which characterizes the density profile in a shallow trap[16]). In contrast with other resummation schemes, such as the large-N expansion[17] or functional renormalization techiques[18], here we treat the normal and anomalous densities on equal footing.

In our approach, we generate a one-parameter family of equivalent Lagrangians. We choose this parameter to reproduce the one-loop result at mean-field level in the weakly-interacting limit. Thus, we identify the optimal auxiliary-field Lagrangian for the purpose of a systematic non-perturbative expansion. Then, the critical temperature variation in leading order is the same as the one found in the next-to-leading order large-N expansion.

In dilute bosonic gas systems, the classical action is given by $S[\,\phi,\phi^*\,] = \int \mathrm{d}x\, \mathcal{L}[\,\phi,\phi^*\,]$, with $\mathrm{d}x \equiv \mathrm{d}t\,\mathrm{d}^3x$ and the Lagrangian density

$$\begin{aligned}\mathcal{L}[\,\phi,\phi^*\,] &= \frac{i\hbar}{2}\,[\,\phi^*(x)\,(\partial_t\,\phi(x)) - (\partial_t\,\phi^*(x))\,\phi(x)\,] \\ &\quad - \phi^*(x)\left\{-\frac{\hbar^2\nabla^2}{2m} - \mu\right\}\phi(x) - \frac{\lambda}{2}\,|\,\phi(x)|^4\,. \end{aligned} \tag{1}$$

Here, μ is the chemical potential and the coupling is $\lambda = 4\pi\hbar^2\,a_0/m$. To account for the contributions of the normal and anomalous densities, we use the Hubbard-Stratonovitch transformation[19] to introduce the real and complex auxiliary fields (AF), $\chi(x)$ and $A(x)$. We add to Eq. (1) the AF Lagrangian density[20, 21]

$$\begin{aligned}\mathcal{L}_{\mathrm{aux}}[\phi,\phi^*,\chi,A,A^*] &= \frac{1}{2\lambda}\left[\,\chi(x) - \lambda\,\cosh\theta\,|\phi(x)|^2\,\right]^2 \\ &\quad - \frac{1}{2\lambda}\left|\,A(x) - \lambda\,\sinh\theta\,\phi^2(x)\,\right|^2, \end{aligned} \tag{2}$$

where θ is the mixing parameter between the normal and anomalous densities, $\chi(x)$ and $A(x)$. The usual large-N approximation[21] is obtained when $\theta = 0$. Then, the action becomes

$$\begin{aligned} S[\Phi,J] &= S[\phi_a,\chi,A,A^*,j_a,s,S] \\ &= -\frac{1}{2}\iint \mathrm{d}x\,\mathrm{d}x'\,\phi_a(x)\,G^{-1\,a}{}_b[\chi,A](x,x')\,\phi^b(x') \\ &\quad + \int \mathrm{d}x\,\Big\{\,\big[\,\chi^2(x) - |A(x)|^2\,\big]/(2\lambda) - s(x)\chi(x) \\ &\quad + S^*(x)A(x) + S(x)A^*(x) + j^*(x)\phi(x) + j(x)\phi^*(x)\,\Big\}\,, \end{aligned} \tag{3}$$

with

$$
\begin{aligned}
G^{-1a}{}_b[\chi, A] &= \left\{ G_0^{-1a}{}_b + V^a{}_b[\chi, A](x) \right\} \delta(x, x') \ , \\
G_0^{-1a}{}_b &= \begin{pmatrix} h_0 & 0 \\ 0 & h_0^* \end{pmatrix} \ , \quad h_0 = -\frac{\hbar^2 \nabla^2}{2m} - i\hbar \frac{\partial}{\partial t} - \mu \ , \\
V^a{}_b[\chi, A](x) &= \begin{pmatrix} \chi(x) \cosh\theta & -A(x) \sinh\theta \\ -A^*(x) \sinh\theta & \chi(x)\cosh\theta \end{pmatrix} \ .
\end{aligned}
\tag{4}
$$

Here, we introduced a two-component notation with $\phi^a(x) = \{\, \phi(x), \phi^*(x) \,\}$ for $a = 1, 2$. $\Phi(x)$ and $J(x)$ signify the five-component fields and currents. The generating functional for connected graphs is

$$
Z[J] = e^{iW[J]/\hbar} = \mathcal{N} \int \mathrm{D}\Phi \, e^{iS[\Phi;J]/\hbar} \ ,
$$

with $S[\Phi; J]$ given by Eq. (3). Performing the path integral over the fields ϕ_a, we obtain the effective action

$$
\begin{aligned}
\epsilon \, S_{\text{eff}}[\chi; J, \epsilon] = \frac{1}{2} \iint \mathrm{d}x \, \mathrm{d}x' \, j_a(x) \, G[\chi]^a{}_b(x, x') \, j^a(x) \\
+ \int \mathrm{d}x \left\{ \frac{\chi_i(x) \, \chi^i(x)}{2\lambda} - S_i(x) \, \chi^i(x) - \frac{\hbar}{2i} \mathrm{Tr} \, \ln[\, G^{-1} \,] \right\} ,
\end{aligned}
$$

where $\chi^i(x) = \left\{ \chi(x), A(x)/\sqrt{2}, A^*(x)/\sqrt{2} \right\}$, $S^i(x) = \left\{ s(x), S(x)/\sqrt{2}, S^*(x)/\sqrt{2} \right\}$. The small parameter ϵ allows us to perform the remaining path integral over χ^i using the stationary-phase approximation. As shown in Ref.20, ϵ counts loops in the AF propagator in analogy with $\hbar$, and provides the loop expansion of the effective action in terms of χ propagators. Next, we expand the effective action about the stationary points, $\chi_0^i(x)$, defined by $\delta S_{\text{eff}}[\chi; j]/\delta\chi_i(x) = 0$. Hence, we obtain

$$
\begin{aligned}
\frac{\chi_0(x)}{\lambda} &= \left\{ \, |\phi_0(x)|^2 + \frac{\hbar}{2i} \, \mathrm{Tr}[\, G(x, x) \,] \, \right\} \cosh\theta + s(x) \ , \\
\frac{A_0(x)}{\lambda} &= \left\{ \, \phi_0^2(x) + \frac{\hbar}{i} \, G^2{}_1(x, x) \, \right\} \sinh\theta + S(x) \ ,
\end{aligned}
$$

where we introduced the notations

$$
\phi_0^a[\chi_0](x) = \int \mathrm{d}x' \, G[\chi_0]^a{}_b(x, x') \, j^b(x') \ .
$$

We emphasize that both χ_0 and A_0 include self-consistent fluctuations. Expanding the effective action about the stationary point, we write

$$S_{\text{eff}}[\chi; J] = S_{\text{eff}}[\chi_0; J] + \frac{1}{2} \iint \mathrm{d}^4x \, \mathrm{d}^4x' \, D^{-1}_{ij}[\chi_0](x, x') \times [\chi^i(x) - \chi^i_0(x)] \, [\chi^j(x') - \chi^j_0(x')] + \cdots \, , \tag{5}$$

where $D^{-1}_{ij}(x, x')$ is given by the second-order derivatives,

$$D^{-1}_{ij}[\chi_0](x, x') = \frac{\delta^2 \, S_{\text{eff}}[\chi^a]}{\delta\chi^i(x) \, \delta\chi^j(x')} \bigg|_{\chi_0} \, ,$$

evaluated at the stationary points. By keeping the gaussian fluctuations and Legendre transforming, the one-particle irreducible (1-PI) graphs generating functional

$$\begin{aligned} \Gamma[\Phi] &= \int \mathrm{d}x \, j_\alpha(x) \, \phi^\alpha(x) - W[J] \qquad (6) \\ &= \frac{1}{2} \iint \mathrm{d}x \, \mathrm{d}x' \, \phi_a(x) \, G^{-1}[\chi]^a{}_b(x, x') \, \phi^b(x') \\ &\quad - \int \mathrm{d}x \, \Big\{ \frac{\chi_i(x) \, \chi^i(x)}{2\lambda} - \frac{\hbar}{2i} \mathrm{Tr} \big\{ \ln[\, G^{-1}[\chi](x, x) \,] \big\} \\ &\qquad - \frac{\hbar \, \epsilon}{2i} \, \mathrm{Tr} \, \ln[\, D^{-1}_{ii}[\Phi](x, x) \,] \Big\} + \cdots \, , \end{aligned}$$

is the negative of the classical action plus self-consistent one-loop corrections in the ϕ_a and χ_i propagators.

To leading order in the AF loop expansion (LOAF), one sets $\epsilon = 0$ in the right-hand-side of (6). The static part of the effective action per unit volume is

$$V_{\text{eff}}[\Phi] = (\chi \cosh\theta - \mu \,) \, |\phi|^2 - \frac{1}{2} \, (A^* \, \phi^2 + A \, \phi^{*\,2}) \sinh\theta - \frac{\chi^2 - |A|^2}{2\lambda} + \frac{\hbar}{2i} \mathrm{Tr} \big\{ \ln[\, G^{-1}[\chi] \,] \big\} \, . \tag{7}$$

Translating (7) to the imaginary time formalism, we find

$$\frac{\hbar}{2i} \mathrm{Tr} \, \ln[\, G^{-1}[\chi] \,] = \int \frac{\mathrm{d}^3k}{(2\pi)^3} \, \Big\{ \frac{\omega_k}{2} + \frac{1}{\beta} \, \ln[\, 1 - e^{-\beta\omega_k} \,] \Big\} \, ,$$

where $\omega_k^2 = (\epsilon_k + \chi \, \cosh\theta - \mu)^2 - |A|^2 \sinh^2\theta$ and $\epsilon_k = k^2/(2m)$. At the minimum, we have

$$\frac{\delta V_{\text{eff}}[\Phi]}{\delta\phi^*} \bigg|_{\phi_0} = (\chi \cosh\theta - \mu) \, \phi_0 - A \, \sinh\theta \, \phi^*_0 = 0 \, . \tag{8}$$

Using the $U(1)$ gauge symmetry, we choose ϕ_0 to be real. Then, A is real and the dispersion, $\omega_k^2 = \epsilon_k(\epsilon_k + 2A \sinh\theta)$, represents the Goldstone theorem. Next, we set $\sinh\theta = 1$, such that

ω_k reduces to the Bogoliubov dispersion, $\omega_k = \sqrt{\epsilon_k(\epsilon_k + 2\lambda\,\phi_0^2)}$, in the limit of vanishing quantum fluctuations in the anomalous density. We note that the leading-order (LO) in the large-N expansion corresponds to $\theta = 0$. This leads to the noninteracting (NI) dispersion, $\omega_k = \epsilon_k$, and we conclude that the large-N expansion is not a suitable starting point, because it is incompatible with the Bogoliubov spectrum.

Using standard regularization techniques[22], the renormalized effective potential is written as

$$V_{\text{eff}}[\Phi] = \chi'|\phi|^2 - \frac{1}{2}\big(A^*\phi^2 + A\phi^{*\,2}\big) - \frac{(\chi'+\mu)^2}{4\lambda} + \frac{|A|^2}{2\lambda}$$
$$+\int \frac{\mathrm{d}^3k}{(2\pi)^3}\Big[\frac{1}{2}\Big(\omega_k - \epsilon_k - \chi' + \frac{|A|^2}{2\epsilon_k}\Big) + \frac{1}{\beta}\ln(1-e^{-\beta\omega_k})\Big],$$

where $\chi' = \sqrt{2}\chi - \mu$ and $\omega_k^2 = (\epsilon_k + \chi' + |A|)(\epsilon_k + \chi' - |A|)$. The gap equations, obtained from $\delta V_{\text{eff}}[\Phi]/\delta\chi^i = 0$, are

$$\frac{A}{\lambda} = \phi^2 + A\int \frac{\mathrm{d}^3k}{(2\pi)^3}\left\{\frac{1+2n(\omega_k)}{2\omega_k} - \frac{1}{2\epsilon_k}\right\}, \tag{9}$$
$$\frac{\chi'+\mu}{2\lambda} = |\phi|^2 + \int \frac{\mathrm{d}^3k}{(2\pi)^3}\left\{\frac{\epsilon_k+\chi'}{2\omega_k}[1+2n(\omega_k)] - \frac{1}{2}\right\},$$

where $n(\omega_k) = [\exp(\omega_k/k_BT) - 1]^{-1}$ is the Bose-Einstein particle distribution. At the minimum of the effective potential we have, $(\chi'_0 - A_0)\,\phi_0 = 0$, see Eq. (8), and we replace μ by the physical density using $\rho = -\partial V_{\text{eff}}[\Phi_0]/\partial\mu = (\chi'_0 + \mu)/(2\lambda)$. The density is used to rescale Eqs. (9), and the ensuing phase diagram problem depends only on the dimensionless parameter, $\rho^{1/3}a_0$, and the coupling constant becomes $\lambda = 8\pi\,\rho^{1/3}a_0$. In the broken symmetry phase, we have $\chi'_0 = A_0$ and the dispersion relation, $\omega_k^2 = \epsilon_k(\epsilon_k + 2\chi'_0)$. The condensate density is denoted by $\rho_0 = \phi_0^2$. At weak coupling and $T = 0$, our results coincide with the Bogoliubov (one-loop) approximation[14], $\mu = 8\pi\rho a_0\big[1 + (32/3)\sqrt{\rho a_0^3/\pi}\,\big]$.

We compare the LOAF results with the predictions of the Popov bosonic approximation (PA)[23]. PA is generally recognized as an accurate theoretical description of experimental data in weakly-coupled dilute trapped Bose gases[24], as long as the densities of the condensed and noncondensed atoms are comparable with each other. Unfortunately, PA produces an artificial first-order phase transition at T_c. Formally, PA is obtained from Eq. (9) by setting $A_0 = \chi'_0 = \lambda\rho_0$ and neglecting the quantum fluctuations in the anomalous density. With this substitution, the PA dispersion relation reads $\omega_k^2 = \epsilon_k(\epsilon_k + 2\lambda\rho_0)$.

In Fig. 1 we depict the temperature dependence of the normal density χ', and anomalous density, A, at constant $\rho^{1/3}a_0$, as derived using the LOAF and PA approximations. For

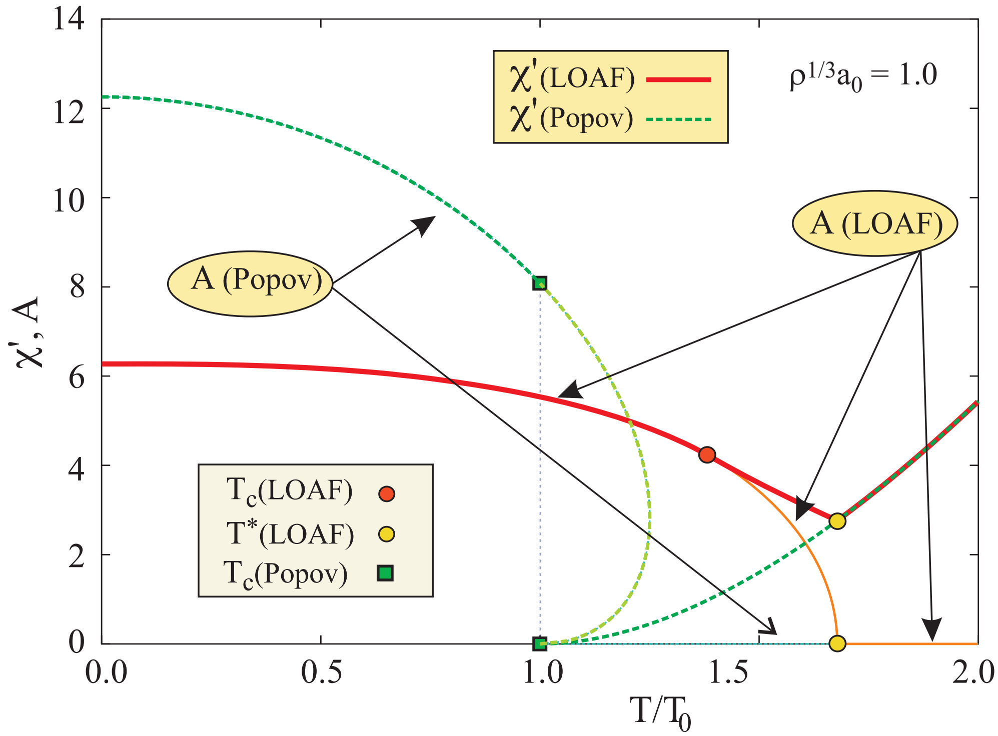

FIG. 1. (Color online) Normal density, χ', and anomalous density, A, from the LOAF and PA approximations, for $\rho^{1/3}a_0 = 1$. T_c and $T^\star$ indicate vanishing condensate density, ρ_0, and anomalous density, A, respectively. PA leads to a first-order phase transition, whereas LOAF predicts a second-order phase transition. We have that $T_c = T^\star$ in the PA, but not in LOAF. In LOAF χ' and A are equal until T_c.

illustrative purposes, we set $\rho^{1/3}a_0 = 1$ and the temperature is scaled by its NI critical value, $T_0 = (2\pi\hbar^2/m)[\rho/\zeta(3/2)]^{2/3}$, where $\zeta(x)$ is the Riemann zeta function. We identify two special temperatures, at T_c where the condensate density vanishes, and at $T^\star$ where the anomalous density, A, vanishes. These temperatures are the same in the PA formalism, but they are different in LOAF. The existence of a temperature range, $T_c < T < T^\star$, for which the anomalous density, A, is nonzero despite a zero condensate fraction, ϕ, is a fundamental prediction of LOAF. In this temperature range, the dispersion relation is expected to depart from the quadratic form predicted by the Popov approximation for $T > T_c$. Above T_c the solution of the PA equations becomes multivalued, indicating that the system undergoes a first-order phase transition at T_c. In contrast, LOAF predicts a second-order transition.

The temperature dependence of the condensate fraction, ρ_0/ρ, is depicted in Fig. 2 for

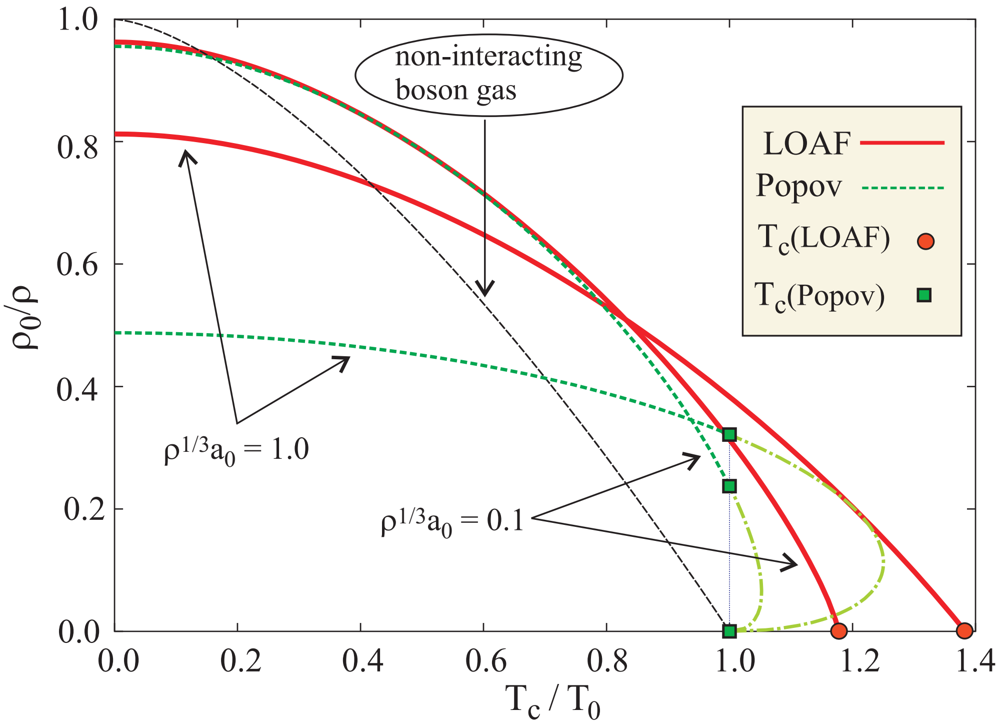

FIG. 2. (Color online) Temperature dependence of the condensate fractions from LOAF and PA, compared with the NI result, for $\rho^{1/3}a_0 = 0.1$ and $\rho^{1/3}a_0 = 1$. Because at T_c the PA and NI dispersion relations are the same, PA does not change T_c relative to the NI case. LOAF increases T_c.

two constant values of the dimensionless parameter $\rho^{1/3}a_0$, together with the NI result, $\rho_0/\rho = 1 - (T/T_0)^{3/2}$. Again, we observe that LOAF exhibits the correct second-order BEC phase transition behavior. Moreover, PA does not change T_c relative to the NI case, because in the PA case we have $T_c = T^\star$ and the PA and NI dispersion relations are the same at T_c. The LOAF approximation predicts an increase of T_c compared with the NI case.

As illustrated in Fig. 2, the LOAF and PA predictions may differ greatly even for temperatures, $T \ll T_c$. These differences are enhanced by a strengthening of the interaction between particles in the Bose gas (a larger value of $\rho^{1/3}a_0$ indicates stronger coupling). The leading-order AF formalism produces a more realistic set of observables away from the weak-coupling limit because of its non-perturbative character. In contrast, PA is appropriate only in the case of a weakly-interacting gas of bosons. The former is made explicit by studying the LOAF prediction for the relative change in T_c with respect to T_0, as a function of $\rho^{1/3}a_0$. The inset in Fig. 3 demonstrates that in the weak-coupling regime, $\rho^{1/3}a_0 \ll 1$, LOAF produces

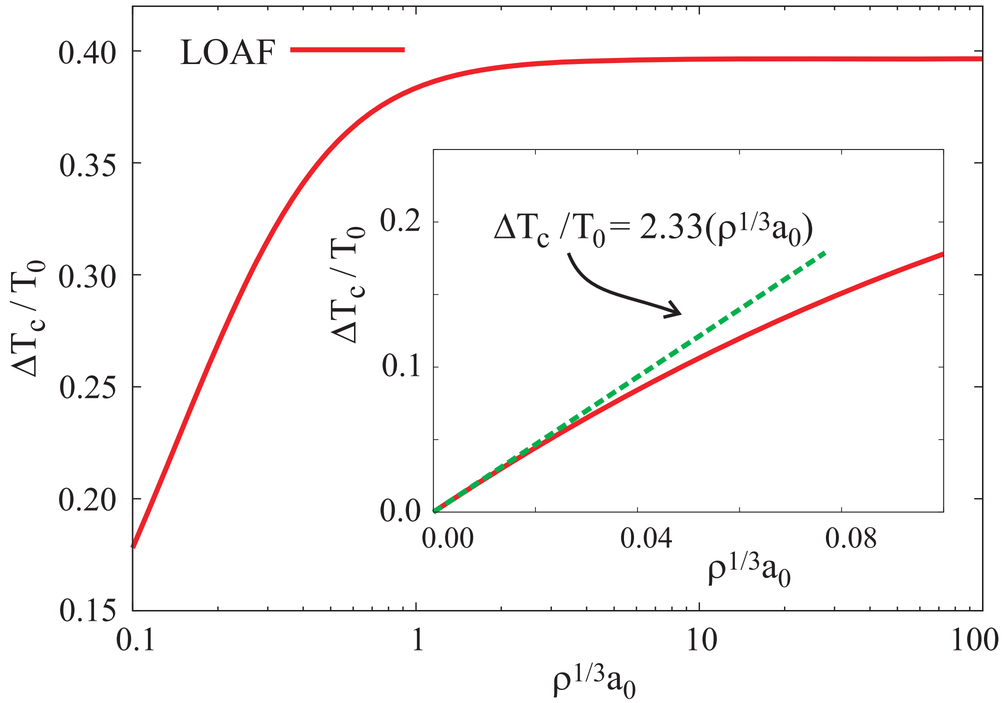

FIG. 3. (Color online) Relative change in T_c with respect to NI, as predicted by LOAF as a function of $\rho^{1/3}a_0$. The inset shows that in the weak-coupling regime, LOAF produces the same slope as the next-to-leading order large-N expansion[17].

the same slope of the linear departure derived by Baym *et al.*[17] using the large-N expansion, but at next-to-leading order. The LOAF corrections to the critical temperature are due to the inclusion of self-consistent fluctuations effects in the mean-field χ' and A densities. A summary of $\Delta T_c/T_0$ theoretical predictions is found in Ref.14. For $\rho^{1/3}a_0 \gg 1$, LOAF predicts that $\Delta T_c/T_0 \to 0.396$ when the system approaches the unitarity limit. Despite that most current experiments probe only the $\rho^{1/3}a_0 \ll 1$ regime, future experiments[11] may access the medium-to-strongly interacting regime, and verify this non-perturbative prediction.

One can systematically improve upon the LOAF approximation by calculating the 1-PI action order-by-order in ϵ. The broken $U(1)$ symmetry Ward identities guarantee Goldstone's theorem order by order in ϵ [20]. For time-dependent problems, however, this expansion is secular[25], and a further resummation is required. The latter is performed using the two-particle irreducible (2-PI) formalism[26]. A practical implementation of this approach is the bare-vertex approximation (BVA)[27]. The BVA is an energy-momentum and particle-number conserving truncation of the Schwinger-Dyson infinite hierarchy of equations obtained by ignoring the derivatives of the self-energy, similarly to the Migdal's theorem[28] approach in condensed matter physics. The BVA proved effective in the case of classical and quantum $\lambda\phi^4$ field theory problems[29] and can be applied to the BEC case.

To summarize, in this paper we introduce a new non-perturbative resummation formulation for the BEC problem. At mean-field level, this approach meets three important criteria for a satisfactory mean-field theory for weakly-interacting bosons[14]: i) the excitation spectrum is gapless (to preserve Goldstone's theorem), ii) LOAF reduces to the known results from Bogoliubov theory at $T = 0$ and weak coupling, and iii) predicts a second-order BEC phase transition. The latter suggests that a AF formulation of the Lagrangian for systems of cold fermionic atoms may also impact the study of the BEC to BCS crossover in dilute fermionic atom systems[30].

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[16] In the Thomas-Fermi approximation, the local BEC density, $\rho(x)$, in a trapping potential, $V_T(x)$, follows from the density-dependent chemical potential, $\mu(\rho) = \mu - V_T(x)$. Taking the gradient of both sides, we find that the local trap force experienced by the bosons $F_T(x) = -\nabla V_T(x)$ and the boson density gradient, $\nabla\rho(x)$, are proportional with a constant of proportionality equal to $\partial\mu/\partial\rho$, related to the compressibility, $\nabla\rho(x)/F_T(x) = \delta\mu/\delta\rho$. With the sensitive density profile measurement developed for fermion thermometry, experimentalists could, in principle, verify the compressibility calculation.

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