Nonperturbative Predictions for Cold Atom Bose Gases with Tunable Interactions

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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 nonperturbative 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 pointlike interacting particles [6].

Unlike liquid helium, cold atoms remain pointlike even when the scattering length is tuned near a Feshbach resonance. Then, strongly correlated cold-atom bosons offer the exciting prospect of studying pointlike strongly interacting bosons, possibly in the universal regime where the scattering length greatly exceeds the interparticle 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 ultracold 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 BECs 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 Letter, 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, and the compressibility (which characterizes the density profile in a shallow trap). In contrast with other resummation schemes, such as the large-N expansion [15] or functional renormalization techniques [16], 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 the mean-field level in the weakly interacting limit. Thus, we identify the optimal auxiliary-field Lagrangian for the purpose of a systematic nonperturbative 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 $S[\phi,\phi^*] = \int dx \mathcal{L}[\phi,\phi^*]$, with $dx \equiv dt d^3x$ and the Lagrangian density

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

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 [17] to introduce the real and complex auxiliary fields (AF) $\chi(x)$ and $A(x)$, respectively. We add to Eq. (1) the AF Lagrangian density [18,19]

$$\mathcal{L}_{\rm aux}[\phi,\phi^*,\chi,A,A^*] = \frac{1}{2\lambda}[\chi(x)-\lambda\cosh\theta|\phi(x)|^2]^2 - \frac{1}{2\lambda}|A(x)-\lambda\sinh\theta\phi^2(x)|^2, \quad (2)$$

where θ is the mixing parameter between the normal and anomalous densities $\chi(x)$ and $A(x)$, respectively. The usual large-N approximation [19] is obtained when $\theta = 0$. Then, the action becomes

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

with

$$G^{-1a}{}_b[\chi,A] = \{G_0^{-1a}{}_b + V^a{}_b[\chi,A](x)\}\delta(x,x'),$$

$$G_0^{-1a}{}_b = \begin{pmatrix} h_0 & 0 \\ 0 & h_0^* \end{pmatrix}, \qquad h_0 = -\frac{\hbar^2\nabla^2}{2m} - i\hbar\frac{\partial}{\partial t} - \mu,$$

$$V^a{}_b[\chi,A](x) = \begin{pmatrix} \chi(x)\cosh\theta & -A(x)\sinh\theta \\ -A^*(x)\sinh\theta & \chi(x)\cosh\theta \end{pmatrix}. \quad (4)$$

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, respectively. The generating functional for connected graphs is

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

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

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

where $\chi^i(x) = \{\chi(x), A(x)/\sqrt{2}, A^*(x)/\sqrt{2}\}$ and $S^i(x) = \{s(x), S(x)/\sqrt{2}, S^*(x)/\sqrt{2}\}$. The small parameter ϵ allows us to perform the remaining path integration over χ^i by using the stationary-phase approximation. As shown in Ref. [18], 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 $\delta S_{\rm eff}[\chi;j]/\delta\chi_i(x) = 0$. Hence, we obtain

$$\frac{\chi_0(x)}{\lambda} = \left\{|\phi_0(x)|^2 + \frac{\hbar}{2i}{\rm Tr}[G(x,x)]\right\}\cosh\theta + s(x),$$

$$\frac{A_0(x)}{\lambda} = \left\{\phi_0^2(x) + \frac{\hbar}{i}G^2{}_1(x,x)\right\}\sinh\theta + S(x).$$

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

$$S_{\rm eff}[\chi;J] = S_{\rm eff}[\chi_0;J] + \frac{1}{2}\iint d^4x d^4x' D_{ij}^{-1}[\chi_0](x,x') \times [\chi^i(x)-\chi_0^i(x)][\chi^j(x')-\chi_0^j(x')] + \cdots, \quad (5)$$

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

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

evaluated at the stationary points. By keeping the Gaussian fluctuations and Legendre transforming, the one-particle irreducible graph generating functional

$$\begin{aligned} \Gamma[\Phi] &= \int dx j_\alpha(x)\phi^\alpha(x) - W[J] \\ &= \frac{1}{2}\iint dx dx' \phi_a(x) G^{-1}[\chi]^a{}_b(x,x')\phi^b(x') \\ &\quad - \int dx\left\{\frac{\chi_i(x)\chi^i(x)}{2\lambda} - \frac{\hbar}{2i}{\rm Tr}\{\ln[G^{-1}[\chi](x,x)]\} \right. \\ &\quad \left. - \frac{\hbar\epsilon}{2i}{\rm Tr}\ln[D_{ii}^{-1}[\Phi](x,x)]\right\} + \cdots \end{aligned} \quad (6)$$

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

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

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

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

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

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

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 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.

By using standard regularization techniques [20], the renormalized effective potential is written as

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

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

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

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 $\rho = -\partial V_{\rm eff}[\Phi_0]/\partial\mu = (\chi_0' + \mu)/(2\lambda)$. The density is used to rescale Eqs. (9); 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]: $\mu = 8\pi\rho a_0[1 + (32/3)\sqrt{\rho a_0^3/\pi}]$.

We compare the LOAF results with the predictions of the Popov bosonic approximation (PA) [21]. The PA is generally recognized as an accurate theoretical description of experimental data in weakly coupled dilute trapped Bose gases [22], as long as the densities of the condensed and noncondensed atoms are comparable with each other. Unfortunately, the PA produces an artificial first-order phase transition at T_c. Formally, the 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 by using the LOAF and PA approximations. For 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

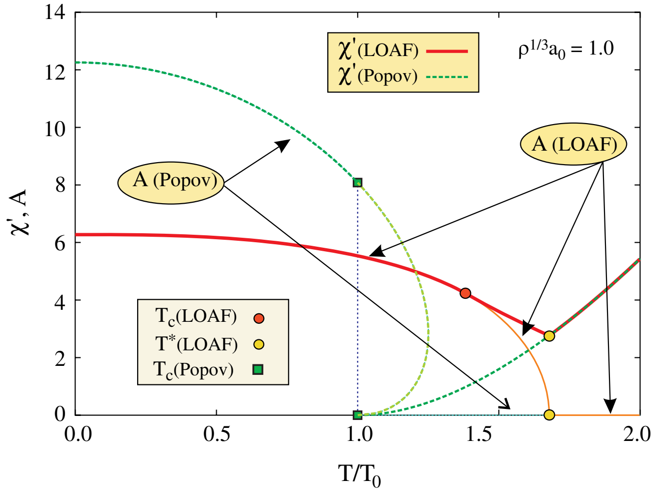

FIG. 1 (color online). Normal density χ' and anomalous density A from the LOAF and PA approximations, for $\rho^{1/3}a_0 = 1$. T_c and $T^\star$ indicate vanishing condensate density ρ_0 and anomalous density A, respectively. The PA leads to a first-order phase transition, whereas the LOAF predicts a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

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 the 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 the 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, the LOAF predicts a second-order transition.

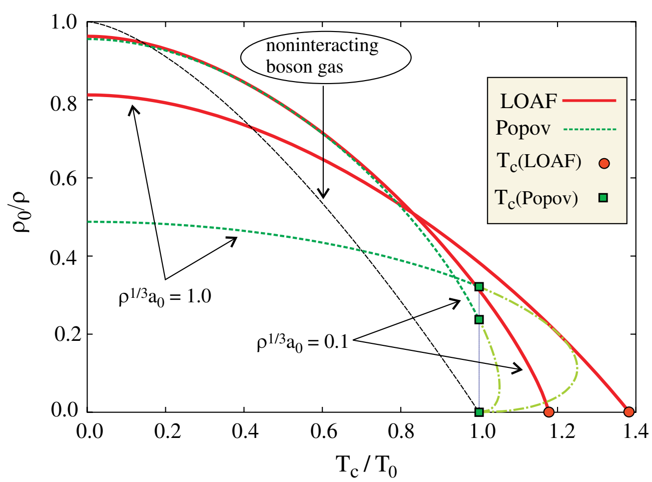

FIG. 2 (color online). Temperature dependence of the condensate fractions from the LOAF and PA, compared with the NI result, for $\rho^{1/3}a_0 = 0.1$ and $\rho^{1/3}a_0 = 1$. Because at T_c the PA and NI dispersion relations are the same, the PA does not change T_c relative to the NI case. The LOAF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

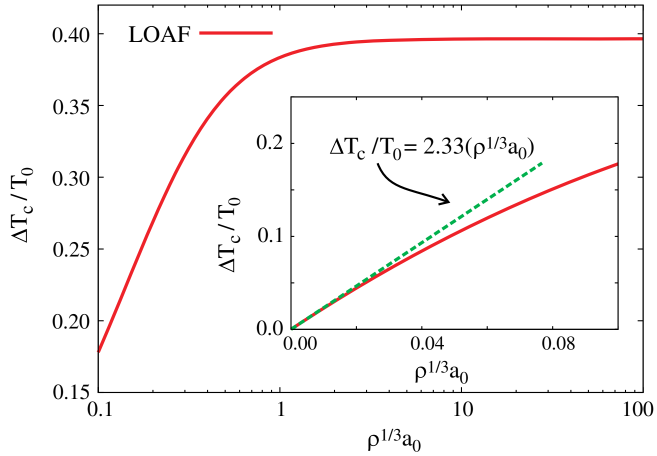

FIG. 3 (color online). Relative change in T_c with respect to NI, as predicted by the LOAF as a function of $\rho^{1/3}a_0$. The inset shows that in the weak-coupling regime, the LOAF produces the same slope as the next-to-leading-order large-N expansion [15].

The temperature dependence of the condensate fraction ρ_0/ρ is depicted in Fig. 2 for 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 the LOAF exhibits the correct second-order BEC phase transition behavior. Moreover, the 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 nonperturbative character. In contrast, the 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, $\rho^{1/3}a_0 \ll 1$, the LOAF produces the same slope of the linear departure derived by Baym, Blaizot, and Zinn-Justin [15] 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 $\rho^{1/3}a_0 \gg 1$, the LOAF predicts that $\Delta T_c/T_0 \to 0.396$ when the system approaches the unitarity limit. Despite the fact 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 nonperturbative prediction.

In summary, in this Letter we introduce a new nonperturbative resummation formulation for the BEC problem. At the 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) the LOAF reduces to the known results from the Bogoliubov theory at $T = 0$ and weak coupling, and (iii) predicts a second-order BEC phase transition.

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