

Improved Self-consistent Mean Field theory for Dilute Bose Gases

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History: A Bose-Einstein condensate (BEC) is a state of matter of a dilute gas of weakly interacting bosons confined in an external potential and cooled to temperatures very near absolute zero. Under such conditions, a large fraction of the bosons occupy the lowest quantum state of the external potential, at which point quantum effects become apparent on a macroscopic scale. This state of matter was first predicted by Satyendra Nath Bose and Albert Einstein in 1924-25. Bose first sent a paper to Einstein on the quantum statistics of light quanta. Einstein was impressed, translated the paper himself from English to German and submitted it for Bose to the *Zeitschrift fur Physik* which published it. Einstein then extended Bose's ideas to material particles (or matter) in two other papers. Seventy years later, the first gaseous condensate was produced by Eric Cornell and Carl Wieman in 1995 at the University of Colorado at Boulder NIST-JILA lab, using a gas of rubidium atoms cooled to 170 nanokelvin (nK)

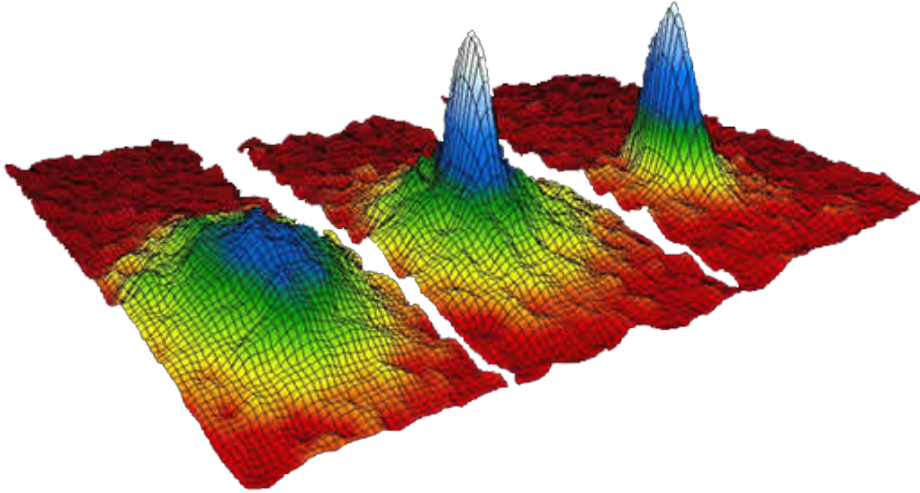


FIG. 1. (Color online) Velocity-distribution data of a gas of rubidium atoms, confirming the discovery of a new phase of matter, the Bose-Einstein condensate. Left: just before the appearance of a Bose-Einstein condensate. Center: just after the appearance of the condensate. Right: after further evaporation, leaving a sample of nearly pure condensate.

I would like to present a new method [1] [2] of introducing composite fields related to the normal and anomalous densities into the effective theory of dilute Bose Gases in a way which preserves Goldstone’s theorem. In leading order one finds

- At weak coupling it reproduces the well known Bogoliubov results and spectrum [3] $\omega_k = \sqrt{k^2(k^2 + 2\lambda v^2)}$
- It has a phonon spectrum to all orders in the expansion parameter (i.e. Goldstone’s theorem)
- It has the correct order of the phase transition to the unbroken symmetry phase (second order phase transition).
- One obtains $\Delta T_c/T_0 = 2.33(\rho^{1/3}a_0)$ in weak coupling
- It predicts a new regime $T_c < T < T^*$ where superfluidity is due to diatom Goldstone condensates
- Using a “gedanken experiment” related to the Higgs Mechanism we can relate the superfluid density ρ_s to the square of the anomalous density [4] .
- For the Bose-Hubbard model one finds [5] a quantum phase transition to the Mott insulator phase

I. REVIEW OF VARIOUS MEAN FIELD THEORY APPROXIMATIONS

Dilute gases can be described by the s-wave scattering amplitude a_s or equivalently by a local 4-boson interaction $(\phi^\star\phi)^2$. Thus the operator equation of motion for the many body field ϕ is

$$\left[-i\hbar \frac{\partial}{\partial t} - \frac{\hbar^2 \nabla^2}{2m} - \mu \right] \phi(x) + \lambda \phi^\star \phi(x) \phi(x) = 0. \quad (1)$$

Taking the expectation of this with respect to the initial density matrix we find we need to evaluate

$$\lambda \langle \phi^\star \phi \phi \rangle \quad (2)$$

Introduce the two composite fields: $\chi = \lambda \phi^\star \phi$ and $A = \lambda \phi \phi$. The Hartree-Fock-Bogoliubov approximation is to replace this by

$$\lambda (2 \langle \phi^\star \phi \rangle \langle \phi \rangle + \langle \phi^\star \rangle \langle \phi \phi \rangle) = 2 \langle \chi \rangle \langle \phi \rangle + \langle \phi^\star \rangle \langle A \rangle \quad (3)$$

However this approximation violates Goldstone's theorem by a term proportional to $\langle (A - \langle A \rangle)^2 \rangle$. Popov [6] sets this term to zero, and obtains Bogoliubov's (one loop) result at weak coupling. BUT also no shift in T_c and a first order phase transition at T_c . Large N (make N copies ϕ_i)

$$\lambda \langle \phi^\star \phi \phi \rangle = \langle \chi \rangle \langle \phi \rangle \quad (4)$$

In leading order large-N the BEC phase is the same as for a free gas. One needs to look at the $1/N$ correction to get the Bogoliubov

spectrum and a shift in T_c [7]. Instead we use the identity:

$$\lambda\phi^*\phi\phi = \chi\phi\cosh^2\theta - \phi^*A\sinh^2\theta \quad (5)$$

In lowest order in the Auxiliary Field loop expansion (LOAF)

$$\lambda\langle\phi^*\phi\phi\rangle = \langle\chi\rangle\langle\phi\rangle\cosh^2\theta - \langle\phi^*\rangle\langle A\rangle\sinh^2\theta \quad (6)$$

For $\sinh\theta = 1$ we reproduce at weak coupling the results of Bogoliubov theory (one loop) [8].

II. BOSE EINSTEIN CONDENSATION IN A FREE GAS

For a given $\langle N \rangle$ as we lower the temperature there is a transition temperature T_0 below which particles must condense into the zero momentum state. For the ideal gas

$$\begin{aligned} Z &= \text{Tre}^{-\beta(H-\mu N)} = \sum_{\{n_i\}} \langle n_1 \dots n_\infty | e^{\beta\mu \sum n_i - \sum \epsilon_i n_i} | n_1 \dots n_\infty \rangle \\ &= \sum_{n_i=1}^{\infty} \prod_{i=1}^{\infty} e^{-\beta n_i(\epsilon_i - \mu)} = \prod_{i=1}^{\infty} \frac{1}{1 - e^{-\beta(\epsilon_i - \mu)}} \end{aligned} \quad (7)$$

$$\Omega = -\frac{1}{\beta} \ln Z = \frac{1}{\beta} \sum_i \ln(1 - e^{-\beta(\epsilon_i - \mu)}) \quad (8)$$

The average number of particles is given by

$$\langle N \rangle = -\frac{\partial \Omega}{\partial \mu} = \sum_i \frac{1}{e^{\beta(\epsilon_i - \mu)} - 1} = \sum_i n_i \quad (9)$$

Here n_i is the mean occupation number in the i th state. For the free particle $\epsilon_i = \epsilon(p) = p^2/2m$. In a box $p_i L_i = 2n_i \pi$. For a given $\langle N \rangle$ there is a temperature below which the continuum expression does not have enough particles. The $p = 0$ state is not counted in the continuum expression and needs to be treated separately. In the continuum

$$\sum_i \rightarrow g \int d^3n = gV \int \frac{d^3p}{(2\pi)^3} \quad (10)$$

This is Bose Einstein Condensation transition temperature T_0 . The chemical potential below T_0 is zero. The critical temperature is the solution of : (Here ρ is considered a fixed external parameter).

$$\rho = \langle N \rangle / V = \int \frac{d^3p}{(2\pi)^3} n[\beta_0 \epsilon_p]; \epsilon_p = p^2/2m \quad (11)$$

Performing the integral one obtains:

$$\rho = \frac{g}{4\pi^2} \left(\frac{2mk_b T_0}{\hbar^2} \right)^{3/2} \zeta(3/2) \Gamma(3/2); \quad (12)$$

$$T_0 = \frac{\hbar^2}{2mk_B} \left(\frac{4\pi^2 \rho}{g \Gamma(3/2) \zeta(3/2)} \right)^{2/3} \quad (13)$$

Below T_0 the density of particle not in the condensate is given by

$$\rho = \frac{g}{4\pi^2} \left(\frac{2mk_b T}{\hbar^2} \right)^{3/2} \zeta(3/2) \Gamma(3/2); \quad (14)$$

One determines the number of particles in the condensate from $N_0 = N - \rho V$ so the fraction is given by

$$\frac{\rho_0}{\rho} = 1 - (T/T_0)^{3/2} \quad (15)$$

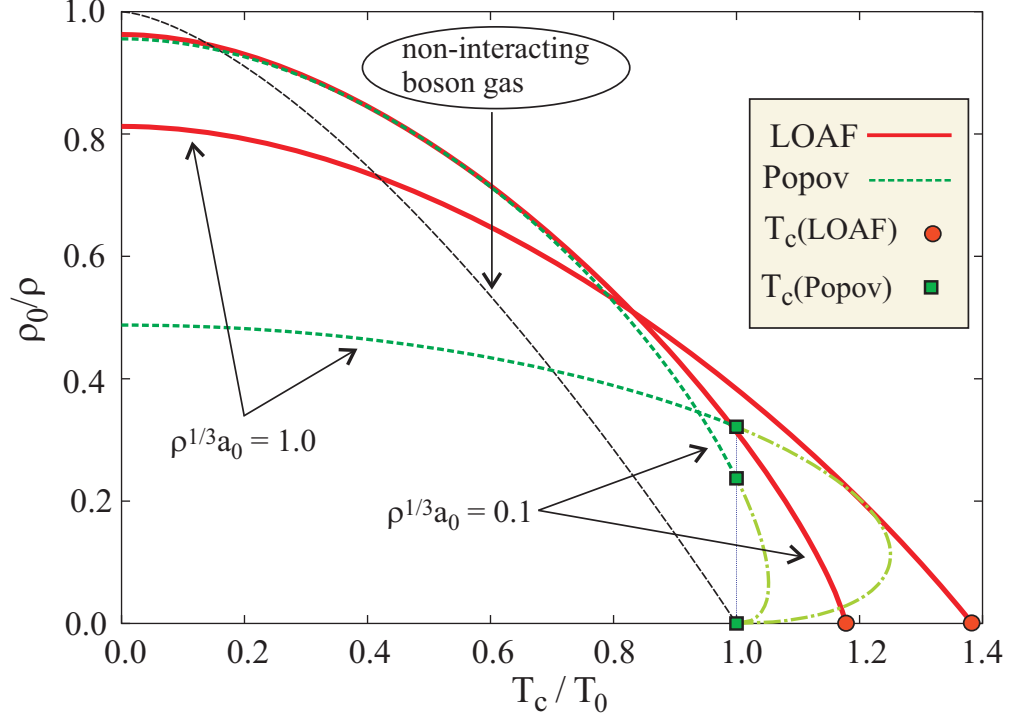


FIG. 2. (Color online) Temperature dependence of the condensate fractions from the LOAF and PA approximations, compared with the NI result, for $\rho^{1/3}a_0 = 0.1$ and $\rho^{1/3}a_0 = 1$. Because at T_c the PA and NI dispersion relations are the same, PA does not change T_c relative to the NI case.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

III. PATH INTEGRAL APPROACH FOR THE FREE GAS

The Grand Partition Function coherent state Path Integral

$$Z = \text{Tre}^{-\beta(H-\mu N)} = \int D\phi^* D\phi e^{-S[\phi^*\phi]} \quad (16)$$

where the action is

$$\begin{aligned} S &= \int_0^\beta d\tau \int d^3x \phi^* \left[\frac{\partial}{\partial \tau} - \nabla^2 - \mu \right] \phi(x, \tau) \\ &= \int_0^\beta d\tau \int d^3x (\phi^\alpha)^*(x, \tau) G_{0,\alpha\beta}^{-1}(x, x'; \tau, \tau') \phi^\beta(x', \tau') \end{aligned} \quad (17)$$

Here $\phi(x, \tau)$ is periodic in τ with period β . $\phi^a(x) = (\phi(x), \phi^*(x))$

Taking the Fourier Transform:

$$\mathcal{G}(x, x') = \frac{1}{\beta} \int \frac{d^3k}{(2\pi)^3} \sum_{n=-\infty}^{+\infty} \tilde{\mathcal{G}}(\mathbf{k}, n) e^{i[\mathbf{k} \cdot (\mathbf{r}-\mathbf{r}') - \omega_n(\tau-\tau')]} . \quad (18)$$

we find that

$$G_0^{-1} = \begin{pmatrix} \epsilon_k - \mu - i\omega_n & 0 \\ 0 & \epsilon_k - \mu + i\omega_n \end{pmatrix} ; G_0 = \begin{pmatrix} \tilde{G}(\mathbf{k}, n) & 0 \\ 0 & \tilde{G}(-\mathbf{k}, -n) \end{pmatrix} \quad (19)$$

where

$$\tilde{G}(\mathbf{k}, n) = \frac{\epsilon_k - \mu + i\omega_n}{\omega_k^2 + \omega_n^2} , \quad (20)$$

Here $\omega_n = 2\pi n/\beta$, $\epsilon_k = k^2/2m$. Performing the Gaussian integral over ϕ one obtains

$$F = -\frac{1}{V\beta} \ln Z = \frac{1}{2} \text{Tr} \ln G^{-1}(\omega_n, p) = \frac{1}{2\beta} \sum_n \int \frac{d^3p}{(2\pi)^3} \ln[\omega_n^2 + (\epsilon_p - \mu)^2] \quad (21)$$

Using

$$\sum_n \ln[\omega_n^2 + \omega^2] = \beta\omega + 2 \ln[1 - e^{-\beta\omega}] \quad (22)$$

We obtain ($\omega_p = \epsilon_p - \mu$)

$$F = \int \frac{d^3p}{(2\pi)^3} \left[\frac{\omega_p}{2} + T \ln[1 - e^{-\beta\omega_p}] \right] \quad (23)$$

The first terms is the vacuum energy term, removing that:

$$F = \int \frac{d^3p}{(2\pi)^3} T \ln[1 - e^{-\beta\omega_p}]. \quad (24)$$

Mean field theory:

- ω now a function of $A(T, \lambda, \rho)$, $\chi(T, \lambda, \rho)$
- A and χ obey self consistent conditions (gap equations)

IV. DILUTE BOSE GAS EFFECTIVE FIELD THEORY AND AUXILIARY FIELD LOOP EXPANSION

For a dilute Bose Gas an effective field theory can be written in terms of a single dimensionless parameter ρa_0^3 , where a_0 is the spin singlet scattering length. The effective action is

$$S[\phi, \phi^*] = \int dx \mathcal{L}[\phi, \phi^*], \quad (25)$$

where $dx := dt d^3x$ and where the Lagrangian density is

$$\begin{aligned} \mathcal{L}[\phi, \phi^*] &= \frac{i\hbar}{2} [\phi^*(x) \partial_t \phi(x) - \partial_t \phi^*(x) \phi(x)] \\ &\quad - \phi^*(x) \left\{ -\frac{\hbar^2 \nabla^2}{2m} - \mu \right\} \phi(x) - \frac{\lambda}{2} |\phi(x)|^4. \end{aligned} \quad (26)$$

Here μ is the chemical potential. $\lambda = 8\pi\hbar^2 a_0/(2m)$. Introduce $\chi(x)$ and $A(x)$ by means of the Hubbard-Stratonovich transformation [9],

$$\begin{aligned} \mathcal{L}_{\text{aux}}[\phi, \phi^*, \chi, A, A^*] &= \frac{1}{2\lambda} [\chi(x) - \lambda \sqrt{2} |\phi(x)|^2]^2 \\ &\quad - \frac{1}{2\lambda} |A(x) - \lambda \phi^2(x)|^2 \end{aligned} \quad (27)$$

which we add to Eq. (26). By doing this the classical action is given by $\mathcal{S}[\Phi] = \int d^4x \mathcal{L}[\Phi]$, where

$$\mathcal{L}[\Phi] = \frac{1}{2\lambda} [\chi^2(x) - |A(x)|^2] - \sqrt{2} \chi(x) |\phi(x)|^2 \quad (28)$$

$$\begin{aligned} &+ [A^*(x)[\phi(x)]^2 + A(x)[\phi^*(x)]^2] \\ &+ \frac{1}{2} [\phi^*(x) h \phi(x) + \phi(x) h^* \phi^*(x)], \\ &h = i\hbar \partial_t + \gamma \nabla^2 + \mu; \quad \gamma = \hbar^2/(2m) \end{aligned} \quad (29)$$

$\Phi^\alpha = (\phi, \phi^*, \chi, A, A^*)$ is a set of five fields. The Lagrangian density possesses a global U(1) symmetry:

$$\phi \rightarrow e^{i\Lambda} \phi, \quad A \rightarrow e^{2i\Lambda} A, \quad (30)$$

Adding sources terms $J^\alpha \Phi_\alpha$, $J^\alpha(x) \equiv (j, j^*, s, S, S^*)$ the generating functional $W[J]$ of connected graphs is

$$Z[J] = e^{iW[J]/\hbar} = \mathcal{N} \int \mathcal{D}\Phi e^{i(\mathcal{S}[\Phi] + \int d^4x J^\alpha(x) \Phi_\alpha(x))},$$

The generator of one-particle irreducible (1-PI) graphs, $\Gamma[\Phi]$, is

$$\Gamma[\Phi] = \int d^4x J^\alpha(x) \Phi_\alpha(x) - W[J], \quad (31)$$

The equations of motion and the inverse propagator are

$$\frac{\delta\Gamma[\Phi]}{\delta\Phi_\alpha(x)} = J_\alpha(x), \quad \frac{\delta^2\Gamma[\Phi]}{\delta\Phi^\alpha(x) \delta\Phi^\gamma(x')} = \mathcal{G}_{\alpha\gamma}^{-1}(x, x'). \quad (32)$$

The path integration over the $\phi(x)$ fields is done exactly and the integral over the fields $\chi(x)$, $A(x)$ and $A^*(x)$ is performed by steepest descent [10]. $S \rightarrow S/\epsilon$. We obtain at leading order in ϵ

$$\begin{aligned} \Gamma[\Phi] = & \frac{1}{2} \iint d^4x d^4x' \phi_a^*(x) G_{ab}^{-1}[\chi, A](x, x') \phi_b(x') \\ & - \int d^4x \left\{ \frac{\chi^2 - |A|^2}{2\lambda} - \frac{\hbar}{2i} \text{Tr}[\ln[G^{-1}[\chi, A](x, x)]] \right\}. \end{aligned}$$

Here, G_{ab}^{-1} represents the $\{1, 2\}$ sector of $\mathcal{G}_{\alpha\beta}^{-1}$, i.e.

$$\begin{aligned} & G_{ab}^{-1}[\chi, A](x, x') \\ & = \delta(x, x') \begin{pmatrix} -i\hbar \partial_t - \gamma \nabla^2 + \chi' & -A \\ -A^* & i\hbar \partial_t - \gamma \nabla^2 + \chi' \end{pmatrix}, \end{aligned} \quad (33)$$

where we introduced the notation $\chi' = \sqrt{2}\chi - \mu$. For the partition function $t \mapsto -i\hbar\tau$. For constant values of χ' and A , we have

$$\mathcal{G}_{\alpha\beta}(x) = \int \frac{d^3k}{(2\pi)^3} \sum_n \tilde{G}_{\alpha\beta}(\mathbf{k}, n) e^{i[\mathbf{k}\cdot\mathbf{r} - \omega_n t]}, \quad (34)$$

where $\omega_n = 2\pi n/T$. From Eq. (33), we find

$$\begin{aligned} \tilde{G}_{11}(\mathbf{k}, n) &= \tilde{G}_{22}^*(\mathbf{k}, n) = \frac{\epsilon_k + \chi' + i\omega_n}{\omega_n^2 + \omega_k^2}, \\ \tilde{G}_{12}(\mathbf{k}, n) &= \tilde{G}_{21}^*(\mathbf{k}, n) = \frac{A}{\omega_n^2 + \omega_k^2}, \end{aligned} \quad (35)$$

$$\omega_k^2 = (\epsilon_k + \chi')^2 - |A|^2 = (\epsilon_k + (\chi' - |A|))(\epsilon_k + (\chi' + |A|)), \quad (36)$$

The effective potential at finite temperature is

$$\begin{aligned} V_{\text{eff}}[\Phi] &= \chi'|\phi|^2 - \frac{A^* \phi^2}{2} - \frac{A \phi^{*2}}{2} - \frac{(\chi' + \mu)^2}{4\lambda} \\ &+ \frac{|A|^2}{2\lambda} + \int \frac{d^3k}{(2\pi)^3} \left[\frac{\omega_k}{2} + T \ln(1 - e^{-\beta\omega_k}) \right], \end{aligned} \quad (37)$$

and the particle density is given by $\rho = -\partial V_{\text{eff}}/\partial\mu = (\chi' + \mu)/(2\lambda)$.

Following [1], minimizing V_{eff} with respect to ϕ^* gives

$$\chi'\phi - A\phi^* = 0. \quad (38)$$

Because of the gauge freedom, we can choose ϕ to be real at the minimum. So for $\phi \neq 0$, $A = \chi'$ and

$$\omega_k^2 = (\epsilon_k)(\epsilon_k + 2A) \quad (39)$$

Minimizing with respect to χ' and A and performing μ , λ and vacuum renormalization, we obtain

$$\frac{A}{\lambda} = \rho_0 + A \int \frac{d^3k}{(2\pi)^3} \left\{ \frac{1 + 2n(\omega_k)}{2\omega_k} - \frac{1}{2\epsilon_k} \right\}, \quad (40a)$$

$$\rho = \rho_0 + \int \frac{d^3k}{(2\pi)^3} \left\{ \frac{\epsilon_k + A}{2\omega_k} [1 + 2n(\omega_k)] - \frac{1}{2} \right\}, \quad (40b)$$

where the condensate density is $\rho_0 = \phi_0^2$, $\lambda = 8\pi\hbar^2 a_0/(2m)$ and $n(x) = (e^x - 1)^{-1}$ is the Bose distribution. The phase diagram in the LOAF approximation is depicted in Fig. 3 as a function of the strength of the inter-particle interaction, which is characterized by the dimensionless parameter $\rho^{1/3}a_0$, where a_0 is the s-wave scattering length. We notice the presence of three distinct regions, corresponding to the values of the three LOAF parameters, the usual (atom) BEC condensate density, ρ_0 , and the normal and anomalous auxiliary fields, χ' and A : Here, the critical temperature T_c corresponds to the emergence of the atom BEC condensate, whereas the temperature T^* is related to the onset of superfluidity in the system and the emergence of a diatom condensate, A . The anomalous auxiliary field A represents a second order parameter in the LOAF theory. In the noninteracting limit, T_c and T^* are the same. As the interaction strength increases, the temperature range for which the superfluid is present in the absence of the

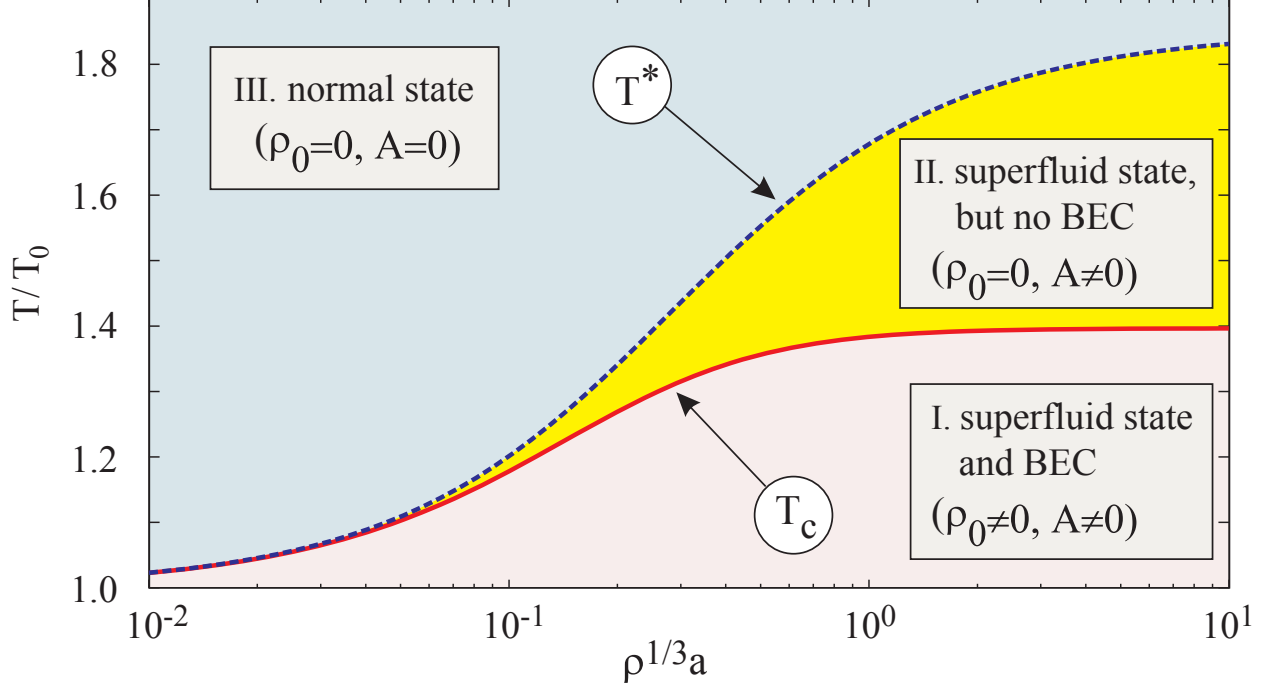


FIG. 3. (Color online) The LOAF phase diagram.

atom BEC condensates expands. LOAF predicts $\sim 20\%$ temperature range $T^* - T_c$ relative to T_c for a dimensionless parameter value, $\rho^{1/3}a = 1$. In regions I and II fields carrying $U(1)$ charge are nonzero, which leads to spontaneous breaking of the $U(1)$ charge and the existence of Goldstone modes. These Goldstone modes are essential for the existence of superfluidity according to the Josephson relationship.

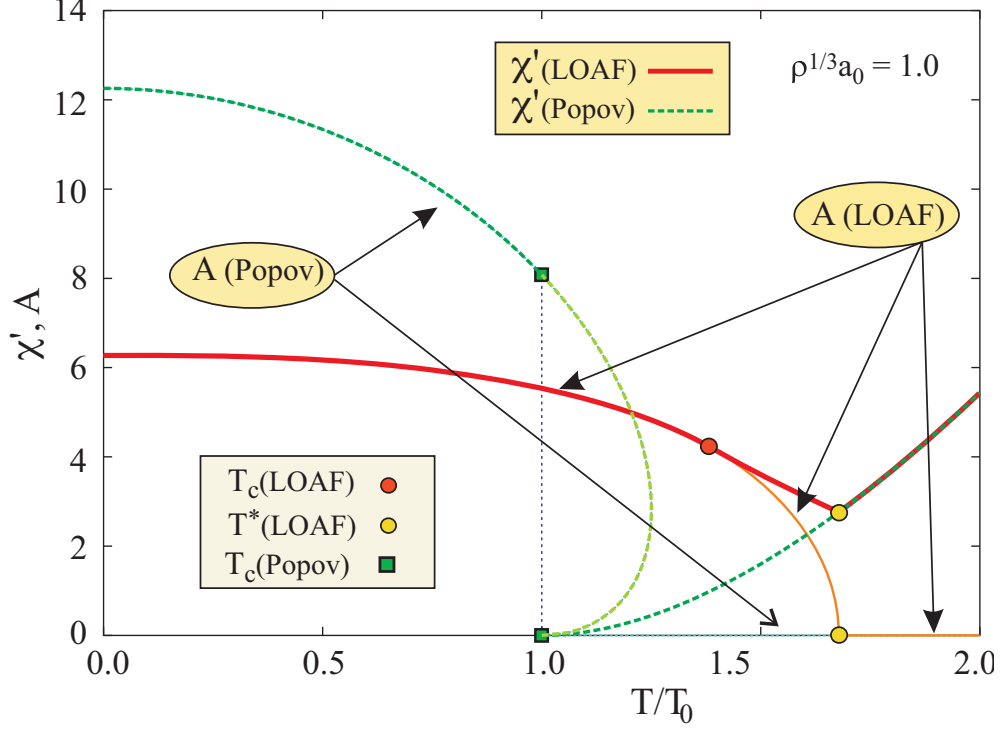


FIG. 4. (Color online) Normal density, χ' , and anomalous density, A , from the LOAF and PA approximations, for $\rho^{1/3}a_0 = 1$. T_c and T^* indicate vanishing condensate density, ρ_0 , and anomalous density, A , respectively. PA leads to a first-order phase transition, whereas LOAF predicts a second-order phase transition. We have that $T_c = T^*$ in the PA, but not in LOAF.

V. HARTREE FOCK BOGOLIUBOV APPROXIMATION

The generating functional $Z[j]$ is written as a path integral,

$$Z[j] = e^{iW[j]/\hbar} = \int D\phi e^{iS[\phi,j]/\hbar}, \quad (41)$$

where $S[\phi, j]$ is the classical action+ sources.

The HFB approximation assumes all fluctuations beyond the second are small, so that the third derivative of W with respect to j is set equal to zero. The connected two-point Green functions are

defined by

$$G[j](x, x') = \frac{\delta^2 W[j]}{\delta j^*(x) \delta j(x')}; K[j](x, x') = \frac{\delta^2 W[j]}{\delta j^*(x) \delta j^*(x')} \quad (42)$$

The Hartree approximation ignores all third-order functional derivatives of $W[j]$ and we obtain

$$\begin{aligned} & \left[-\frac{\hbar^2 \nabla^2}{2m} - i\hbar \frac{\partial}{\partial t} - \mu \right] \phi(x) + \lambda |\phi(x)|^2 \phi(x) \\ & + 2 \frac{\lambda \hbar}{i} G[j](x, x) \phi(x) + \frac{\lambda \hbar}{i} K[j](x, x) \phi^*[j](x) = j(x). \end{aligned} \quad (43)$$

Defining new auxiliary fields $\chi(x)$ and $A(x)$ by,

$$\frac{\chi(x) + \mu}{2\lambda} = |\phi(x)|^2 + \hbar G(x, x)/i, \quad (44a)$$

$$\frac{A(x)}{\lambda} = [\phi(x)]^2 + \hbar K(x, x)/i. \quad (44b)$$

$$\left[h_0 + \chi(x) - 2\lambda |\phi(x)|^2 \right] \phi(x) + A(x) \phi^*(x) = 0.$$

$$h_0 = \frac{\hbar^2 \nabla^2}{2m} - i\hbar \frac{\partial}{\partial t}. \quad (45)$$

Functional differentiation of Eq. (43) w.r.t. $j(x')$ and $j^*(x')$,

$$\left[h_0 + \chi(x) \right] G(x, x') + A(x) K^*(x, x') = \delta(x, x'), \quad (46a)$$

$$\left[h_0 + \chi(x) \right] K(x, x') + A(x) G^*(x, x') = 0, \quad (46b)$$

and the complex conjugates.

The action for HFB

$$\Gamma_{\text{H}}[\phi, \chi, A, A^*] = \int dx \left\{ \phi^*(x) [h_0 + \chi(x)] \phi(x) - \lambda |\phi(x)|^4 - \frac{(\chi + \mu)^2}{4\lambda} \right. \\ \left. - \frac{|A|^2}{2\lambda} + \frac{1}{2} [\phi^2(x) A^*(x) + \phi^{*2}(x) A(x)] + \frac{\hbar}{2i} \ln[\det[\mathcal{G}^{-1}(x, x)]] \right\}, \quad (47)$$

where the terms in **red** are different than in LOAF.

$$\mathcal{G}^{-1}(x, x') = \delta(x, x') \begin{pmatrix} h_0 + \chi(x) & A(x) \\ A^*(x) & h_0^* + \chi(x) \end{pmatrix}. \quad (48)$$

Again calculating the effective potential in the Matsubara formalism we find the dispersion relation:

$$\omega_k^2 = (\epsilon_k + \chi)^2 - |A|^2 = (\epsilon_k + \chi + |A|) (\epsilon_k + \chi - |A|). \quad (49)$$

The minimum of the potential is when

$$\left. \frac{\partial V_{\text{H}}}{\partial \phi^*} \right|_{\phi_0} = \chi_0 \phi_0 - 2\lambda |\phi_0|^2 \phi_0 + A_0 \phi_0^* = 0, \quad (50)$$

So for the broken symmetry case when $\phi_0 \neq 0$, we have

$$\chi_0 + A_0 = 2\lambda |\phi_0|^2. \quad (51)$$

At the minimum of the effective potential, the dispersion relation **(50)** is

$$\omega_k^2 = [\epsilon_k + 2\lambda |\phi_0|^2] [\epsilon_k - 2(A_0 - \lambda |\phi_0|^2)]. \quad (52)$$

The self-consistency conditions are:

$$\rho = -\frac{\partial V_H}{\partial \mu} = \frac{\chi_0 + \mu}{2\lambda} = \rho_0 + \int \frac{d^3k}{(2\pi)^3} \left\{ \frac{\epsilon_k + \chi_0}{2\omega_k} [1 + 2n(\omega_k)] - 1 \right\}. \quad (54)$$

Here we have set $\rho_0 = \phi_0^2$ which is the condensate density. We also have

$$\frac{A_0}{\lambda} = \rho_0 - A_0 \int \frac{d^3k}{(2\pi)^3} \left\{ \frac{1}{2\omega_k} [1 + 2n(\omega_k)] - \frac{1}{2\epsilon_k} \right\}, \quad (55)$$

where ω_k is given in Eq. (53).

We solve Eqs. (54) and (55) for ρ_0/ρ as a function of T/T_0 , with ω_k given by Eq. (53). The Hartree approximation is compared to LOAF and Popov in Fig. 8

VI. POPOV APPROXIMATION

Because the breakdown of the Goldstone theorem is due to the fluctuation term in A , Popov set this term equal to zero [6]. Requiring

$$A = \lambda \langle \phi \rangle^2 \quad (56)$$

Thus one obtains a gapless spectrum at the cost of an artificial first-order phase transition and no shift in the critical temperature. .

The the dispersion relation is $\omega_p = p\sqrt{p^2 + 2\lambda v^2}$. There is only

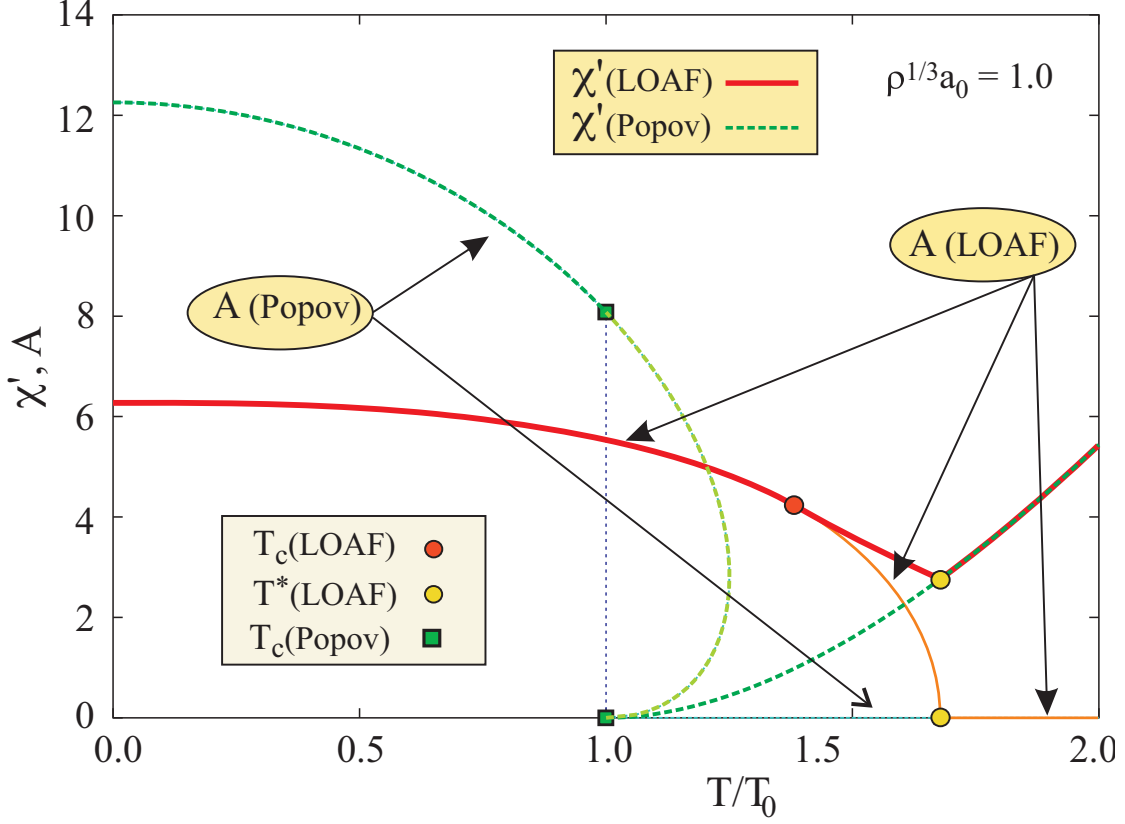


FIG. 5. (Color online) Normal density, χ' , and anomalous density, A , from the LOAF and PA approximations, for $\rho^{1/3}a_0 = 1$. T_c and T^* indicate vanishing condensate density, ρ_0 , and anomalous density, A , respectively. PA leads to a first-order phase transition, whereas LOAF predicts a second-order phase transition. We have that $T_c = T^*$ in the PA, but not in LOAF.

one self-consistent equation for ρ_0 .

$$\rho = \rho_0 + \frac{\sqrt{2}}{12\pi^2}(\lambda\rho_0)^{3/2} + \frac{1}{4\pi^2} \int dp \frac{p^2[p^2 + \omega_p^2/p^2]}{\omega_p} n(\omega_p).$$

VII. NUMERICAL RESULTS

When we compare the free gas result with the LOAF, POPOV and Hartree-Fock Bogoliubov approximations, we find that LOAF overcomes the difficulties of both the Popov (1st order Transition, no shift in T_c), Hartree (not gapless, no shift in T_c and a 1st order transition). The anomalous density leads to a new temperature regime $T_c < T < T^*$ where T_c is where $\phi \rightarrow 0$ and T^* where $A \rightarrow 0$.

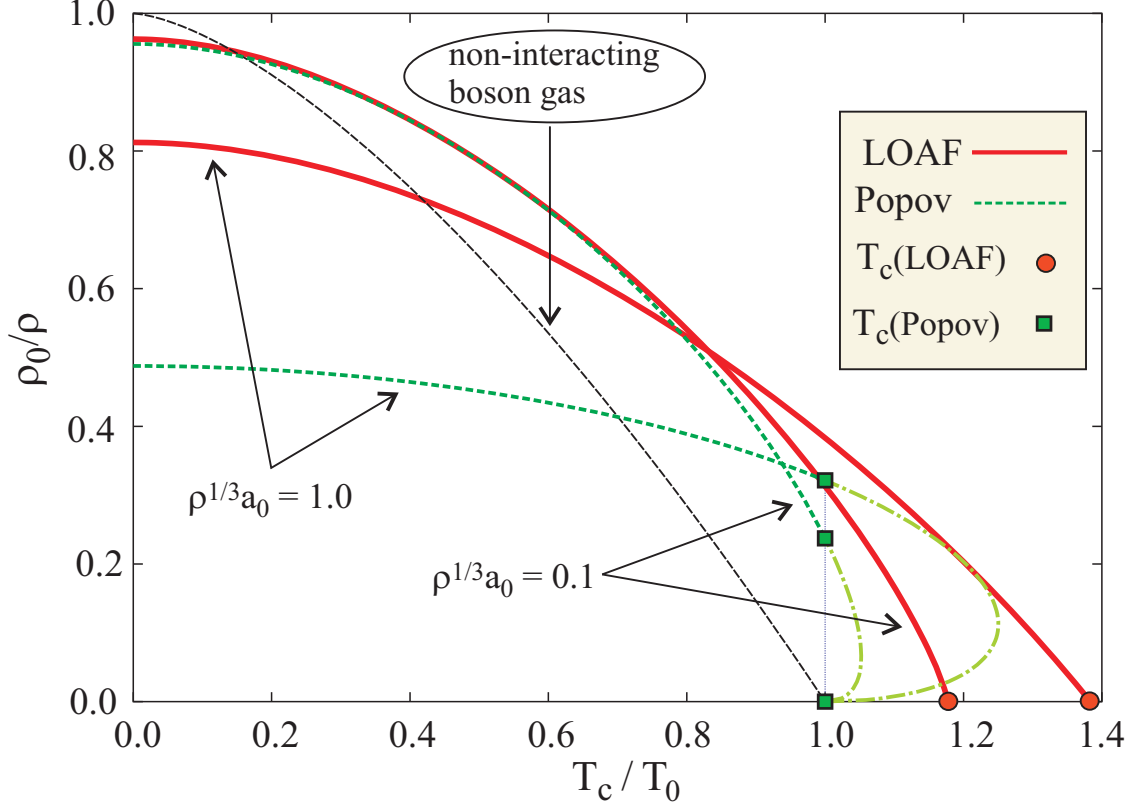


FIG. 6. (Color online) Temperature dependence of the condensate fractions from the LOAF and PA approximations, compared with the NI result, for $\rho^{1/3}a_0 = 0.1$ and $\rho^{1/3}a_0 = 1$. Because at T_c the PA and NI dispersion relations are the same, PA does not change T_c relative to the NI case. LOAF increases T_c .

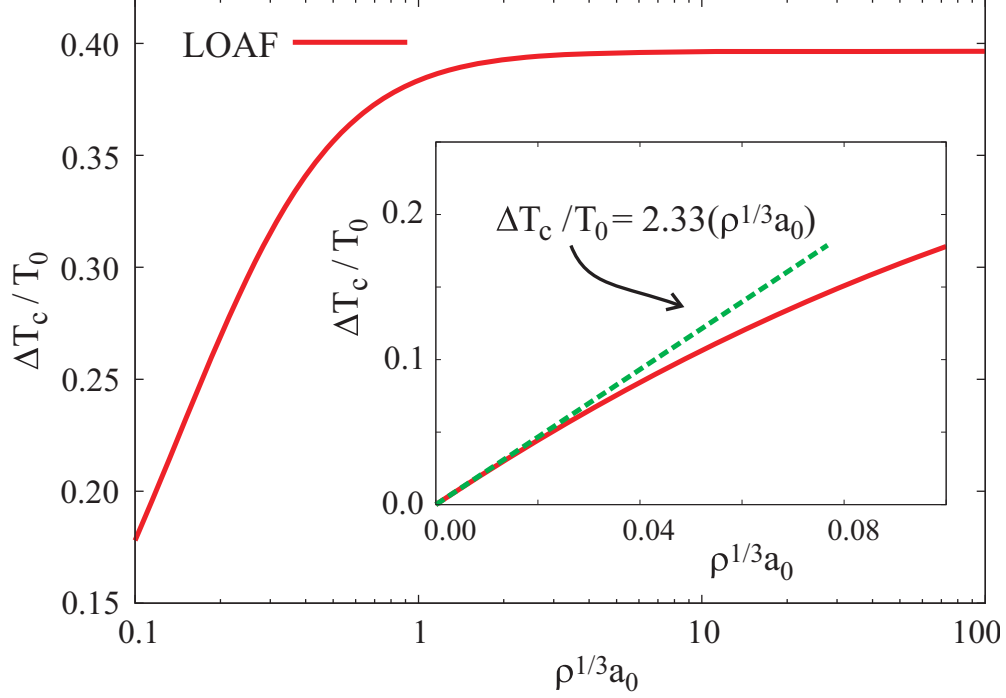


FIG. 7. (Color online) Relative change in T_c with respect to NI, as predicted by LOAF as a function of $\rho^{1/3}a_0$. The inset shows that in the weak-coupling regime, LOAF produces the same slope as the NLO large-N expansion[7].

VIII. JOSEPHSON RELATION- ORDER PARAMETER FOR SUPERFLUIDITY

We want to show that superfluidity requires Goldstone modes and that in LOAF these are also in the correlation function for the composite field A . We will find either by direct computation[11] or by a Gedanken experiment [4] that in the LOAF approximation

$$\rho_s \propto A^2 \quad (57)$$

Consider a superfluid moving with velocity \mathbf{v} in the laboratory frame. The Lagrangian for this system is obtained by replacing

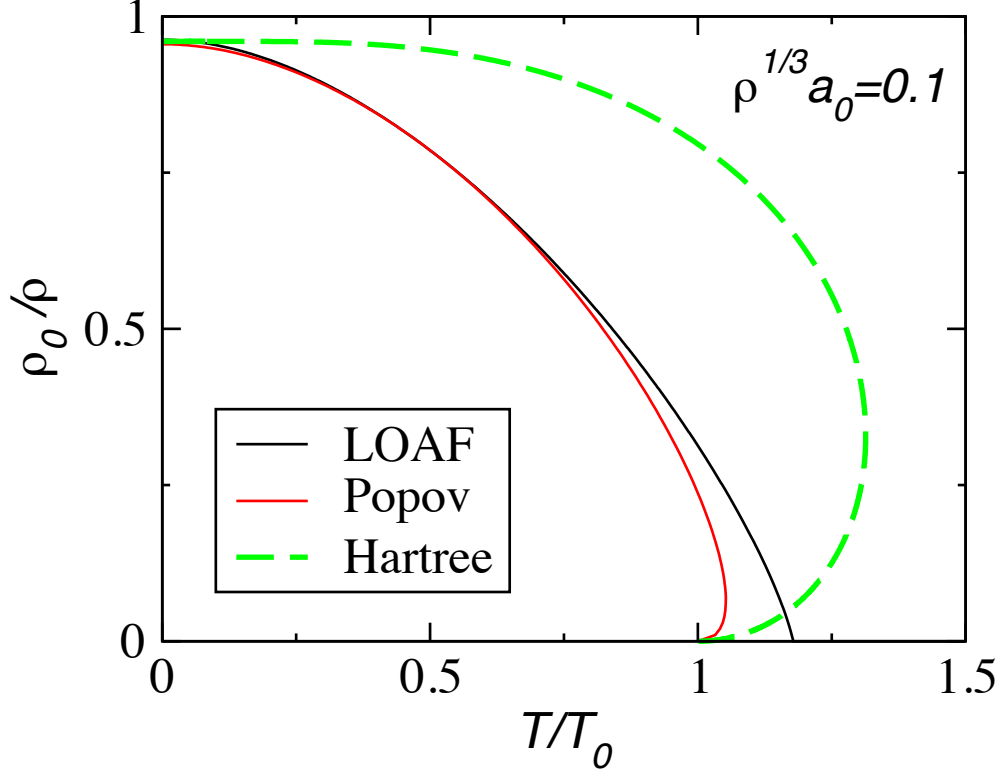


FIG. 8. Comparison of ρ_0/ρ for LOAF (black solid lines), Popov (red solid lines), and Hartree (green dash lines) approximations for $\rho^{1/3}a_0 = 0.1$. ρ_0/ρ

the momentum operator for the system at rest by

$$\frac{\hbar}{i} \nabla \mapsto \mathbf{P} \equiv \frac{\hbar}{i} \nabla - m \mathbf{v} . \quad (58)$$

Then, the superfluid mass density is given by the second-order derivative of the free energy,

$$\rho_s = \frac{1}{V} \left[\frac{\partial^2 F(V, N, T, v)}{\partial v^2} \right]_{v=0} , \quad (59)$$

where v is the velocity of the superfluid. The free energy is related to the grand potential $\Omega(V, \mu, T, v)$ by

$$F(V, N, T, v) = \Omega(V, \mu, T, v) + \mu N . \quad (60)$$

It was shown in Ref. 12 that Eq. (59) is equivalent to

$$\rho_s = \frac{1}{V} \left[\frac{\partial^2 \Omega(v)}{\partial v^2} \right]_{v=0}, \quad (61)$$

which is what we use here.

The shifted action after the Hubbard-Stratonovich transformation is

$$\begin{aligned} S[J, \Phi; \mu, \beta, \mathbf{v}] & \\ &= \frac{1}{2} \iint [dx] [dx'] \phi_a(x) G_v^{-1a}{}_b[\Phi](x, x') \phi^b(x') \\ &+ \int [dx] \left\{ [|A(x)|^2 - \chi^2(x)]/(2\lambda) + J^\alpha(x) \Phi^\alpha(x) \right\}, \end{aligned} \quad (62)$$

where

$$G_v^{-1a}{}_b[\Phi](x, x') = \delta(x, x') \begin{pmatrix} h_v^{(+)} & -A(x) \\ -A^*(x) & h_v^{(-)} \end{pmatrix}, \quad (63)$$

with

$$\begin{aligned} h_v^{(+)} &= h_v + \partial_\tau, & h_v^{(-)} &= h_v^* - \partial_\tau, \\ h_v &= -\frac{\hbar^2 \nabla^2}{2m} - \frac{\hbar}{i} \mathbf{v} \cdot \nabla + \frac{1}{2} m v^2 + \sqrt{2} \chi(x) - \mu. \end{aligned} \quad (64)$$

Computing derivative of the action, we find

$$\frac{\partial S}{\partial v_i} = - \int [dx] j_i(x), \quad (65)$$

where $j_i(x)$ is the classical mass current density,

$$j_i(x) = \frac{\hbar}{2i} \left[\phi^*(x) \nabla_i \phi(x) - \phi(x) \nabla_i \phi^*(x) \right] - v_i \rho(x), \quad (66)$$

with $\rho(x) = |\phi(x)|^2$. The superfluid density is evaluated from the current current correlation function and we found [11] that in LOAF

$$\rho_s = -\frac{8m^2|A|^2}{\hbar^2} \lim_{q \rightarrow 0} \frac{1}{q^2 \tilde{\mathcal{G}}^A_A(q, 0)}. \quad (67)$$

Here, $\tilde{\mathcal{G}}^A_A$ is the Fourier transform of the connected propagator corresponding to the expectation value $\langle A^\star A \rangle$. So we see that we need Goldstone modes in the A propagator to have superfluidity.

This is similar to the Josephson relation for the case of interacting dilute Fermi gases was derived by Taylor which has the form [13]

$$\rho_s = -\frac{m_B^2|\Delta|^2}{\hbar^2} \lim_{q \rightarrow 0} \frac{1}{q^2 \tilde{D}_{11}(q, 0)}, \quad (68)$$

where \tilde{D}_{11} is the Fourier transform of the connected propagator corresponding to the expectation value $\langle \Delta^\star \Delta \rangle$ for quasi-particle bosons of mass, m_B , constructed as pairs of mass m_F fermions ($m_B = 2m_F$). Here the gap parameter, Δ , is the auxiliary field, $\Delta = \langle \psi_\uparrow \psi_\downarrow \rangle$, the propagator D_{11} is an auxiliary-field propagator, similarly to what is described in Eq. (67). The fact that in LOAF the Josephson relation (67) is different from the classical expression [14, 15] is due to the fact that in our auxiliary field formalism, we treat the normal and anomalous density condensate condensates

on equal footing. By doing so we find that the propagator for the composite field A contains a Goldstone excitation.

IX. GOLDSTONE THEOREM- SUPERFLUIDITY-MEISSNER EFFECT-HIGGS PHENOMENA

The superfluid state in the Bose gas is discussed using Landau's phenomenological two-fluid model [16]. We define the normal-state density

$$\rho_n = \frac{1}{3\pi^2} \int_0^\infty dk k^2 \epsilon_k \left[-\frac{\partial n(\omega_k)}{\partial \omega_k} \right], \quad (69)$$

where ω_k is the quasi-particle energy given by the LOAF dispersion relation (36). Correspondingly, the superfluid density is defined as $\rho_s = \rho - \rho_n$. In Fig. 9, we illustrate the temperature dependence of the atom BEC condensate, ρ_0 , and the superfluid density, ρ_s , relative to the system density, ρ , for an interaction strength $\rho^{1/3}a = 0.4$. As advertised, the onset of superfluidity in the system occurs at T^* , and this temperature is different from the T_c , the emergence temperature of the atom BEC condensate.

If we promote the U(1) symmetry to a gauge symmetry by setting $\Lambda \rightarrow g\Lambda(x)/\hbar$ where g is the U(1) charge, in order to preserve the symmetry we introduce a gauge field $W_\mu(x) = (W_0(x), \mathbf{W}(x))$ analogous to the weak interaction vector gauge field. Then, the

boson fields, ϕ , and the anomalous auxiliary field, A , carry one and two units of $U(1)$ charge, respectively. The LOAF approximation predicts that the superfluid state is accompanied by a Meissner effect in the presence of a weak vector potential, $\mathbf{W}(x)$. Following the standard derivation [17] of the supercurrent in BCS theory and adapting it to the case of a Bose gas one finds

$$\mathbf{j}_s(\mathbf{q}) = -\rho_s \frac{g^2}{mc} \mathbf{W}(\mathbf{q}) . \quad (70)$$

where the superfluid density ρ_s in Eq. (70) is the same as that obtained in the Landau two-fluid model:

$$\rho_s = \rho - \frac{1}{3\pi^2} \int_0^\infty dk k^2 \epsilon_k \left[-\frac{\partial n(\omega_k)}{\partial \omega_k} \right] , \quad (71)$$

From the supercurrent (70) and the Maxwell equation, $\nabla \times (\nabla \times \mathbf{W}) = \mathbf{j}_s$, we find the London equation [19]

$$\nabla^2 \mathbf{W} + \frac{c}{4\pi \lambda_L^2} \mathbf{W} = \nabla^2 \mathbf{W} + \frac{\rho_s g^2}{mc} \mathbf{W} = 0 , \quad (72)$$

where $\lambda_L = \sqrt{mc^2/(4\pi\rho_s g^2)}$ is the London penetration depth for the \mathbf{W} field.

A. Composite Field Goldstone Theorem, Higgs Phenomena and order parameter

In region 2 of the phase diagram $\langle \phi \rangle = 0$; $A \neq 0$. A has $U(1)$ charge of two.

The Goldstone theorem (Goldstone 1961) states that when a continuous symmetry, such as $U(1)$, is spontaneously broken, then, necessarily, new massless scalar states appear in the excitation spectrum related to the order parameter. In LOAF, the composite-field Goldstone theorem for the auxiliary field A gives rise to a massless scalar when $T_c < T < T^*$. To derive the Goldstone theorem, one utilizes Noether's theorem for the $U(1)$ transformation (30) on the fields Φ . For constant fields and in the absence of sources one obtains from Noether's theorem $\mathcal{M}_{\alpha\beta} \Phi^\beta = 0$, where $\mathcal{M}_{\alpha\beta}$ is a 4×4 matrix with indices $\{1, 2, 4, 5\}$ for ϕ, ϕ^*, A, A^* and

$$\mathcal{M}_{\alpha\beta} = \int d^4x' \mathcal{G}_{\alpha\gamma}^{-1}(x, x') g^\gamma{}_\beta = \tilde{\mathcal{G}}_{\alpha\gamma}^{-1}(0, 0) g^\gamma{}_\beta. \quad (73)$$

The Goldstone theorem corresponds to $\det[\mathcal{M}] = 0$ and implies the presence of a pole in the propagator at zero-energy and zero-momentum transfer [18] We obtain

$$[\tilde{\mathcal{G}}_{11}^{-1}(0, 0) - \tilde{\mathcal{G}}_{12}^{-1}(0, 0)] \phi = 0, \quad \text{BEC region} \quad (74)$$

$$[\tilde{\mathcal{G}}_{4,4}^{-1}(0, 0) - \tilde{\mathcal{G}}_{5,4}^{-1}(0, 0)] A = 0. \quad \text{Region 2} \quad (75)$$

The Goldstone theorem for the atom BEC condensate corresponds to the case $\phi \neq 0$. Hence, Eq. (74) is consistent with the minimum condition (38), in region I : for $T < T_c$ with $\chi' = A$. In LOAF in

general

$$\begin{aligned} & \tilde{\mathcal{G}}_{4,4}^{-1}(0,0) - \tilde{\mathcal{G}}_{4,5}^{-1}(0,0) \\ &= \frac{1}{2} \left[\frac{1}{\lambda} - \int \frac{d^3k}{(2\pi)^3} \frac{1 + 2n(\omega_k/T)}{2\omega_k} \right] = \frac{\rho_0}{2A}. \end{aligned} \quad (76)$$

Here we used

$$\begin{aligned} \tilde{\mathcal{G}}_{4,4}^{-1}(0,0) &= \frac{1}{2\lambda} + \frac{T}{2} \int \frac{d^3k}{(2\pi)^3} \sum_n \tilde{G}_{11}(\mathbf{k}, n) \tilde{G}_{22}(\mathbf{k}, n), \\ \tilde{\mathcal{G}}_{4,5}^{-1}(0,0) &= \frac{T}{2} \int \frac{d^3k}{(2\pi)^3} \sum_n \tilde{G}_{12}(\mathbf{k}, n) \tilde{G}_{12}(\mathbf{k}, n), \end{aligned}$$

In region II ($T_c < T < T^*$) ρ_0 is zero but $A \neq 0$, Eq. (76) is identically zero and we find a composite-field Goldstone theorem, corresponding to a zero energy and momentum excitation of the gas.

To relate ρ_s to the fundamental quantities of our theory, we note that the $\text{Tr}\{\ln G^{-1}\}$ term in the action leads to nonlocal temperature-dependent $n-A$ vertices. The relativistic effective field theory for the field \mathcal{A} in the presence of a U(1) gauge field has the form

$$\mathcal{L} = (D_\mu \mathcal{A})^* (D^\mu \mathcal{A}) - \lambda_A (|\mathcal{A}|^2 - A^2)^2 - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}, \quad (77)$$

with the covariant derivative, $D_\mu = \partial_\mu + 2igW_\mu$, and $F_{\mu\nu} = \partial_\mu W_\nu - \partial_\nu W_\mu$. Here, $\lambda_A \equiv \lambda_A(T)$ is the value of the four-point field

interaction at zero momentum transfer and temperature T , and $A \equiv A(T)$ is obtained by solving Eqs. (40a) and (40b) for $T < T^*$. Note that when $g \rightarrow 0$, this is the usual effective Lagrangian for charged scalars which exhibits the Goldstone theorem. Letting

$$\mathcal{A} = A + \frac{1}{\sqrt{2}} (\mathcal{A}_1 + i\mathcal{A}_2), \quad \langle \mathcal{A}_1 \rangle = \langle \mathcal{A}_2 \rangle = 0, \quad (78)$$

And introducing a new field: $W'_\mu = W_\mu + \partial_\mu \mathcal{A}_2 / (2\sqrt{2} g A)$,

$$\begin{aligned} \mathcal{L} = & \frac{1}{2}(\partial_\mu \mathcal{A}_1)^2 - \frac{1}{2} \lambda_A A^2 \mathcal{A}_1^2 - \frac{1}{4} F'_{\mu\nu} F'^{\mu\nu} \\ & + (2gA)^2 W'_\mu W'^\mu + \dots \end{aligned} \quad (79)$$

where $F'_{\mu\nu} = \partial_\mu W'_\nu - \partial_\nu W'_\mu$. Hence, the field \mathcal{A}_1 has a composite-field Higgs mass, $M_H^2 = \lambda_A A^2$, whereas the effective mass of the gauge field W'_μ is $M_W^2 = (2g A)^2$. The latter is identified as

$$M_W^2 = (2g A)^2 \longrightarrow \rho_s \frac{g^2}{mc^2}. \quad (80)$$

This implies that A^2 is a measure of the superfluid density, ρ_s . In Fig. 9 we show the temperature dependence of A^2 closely resembles that of the superfluid density.

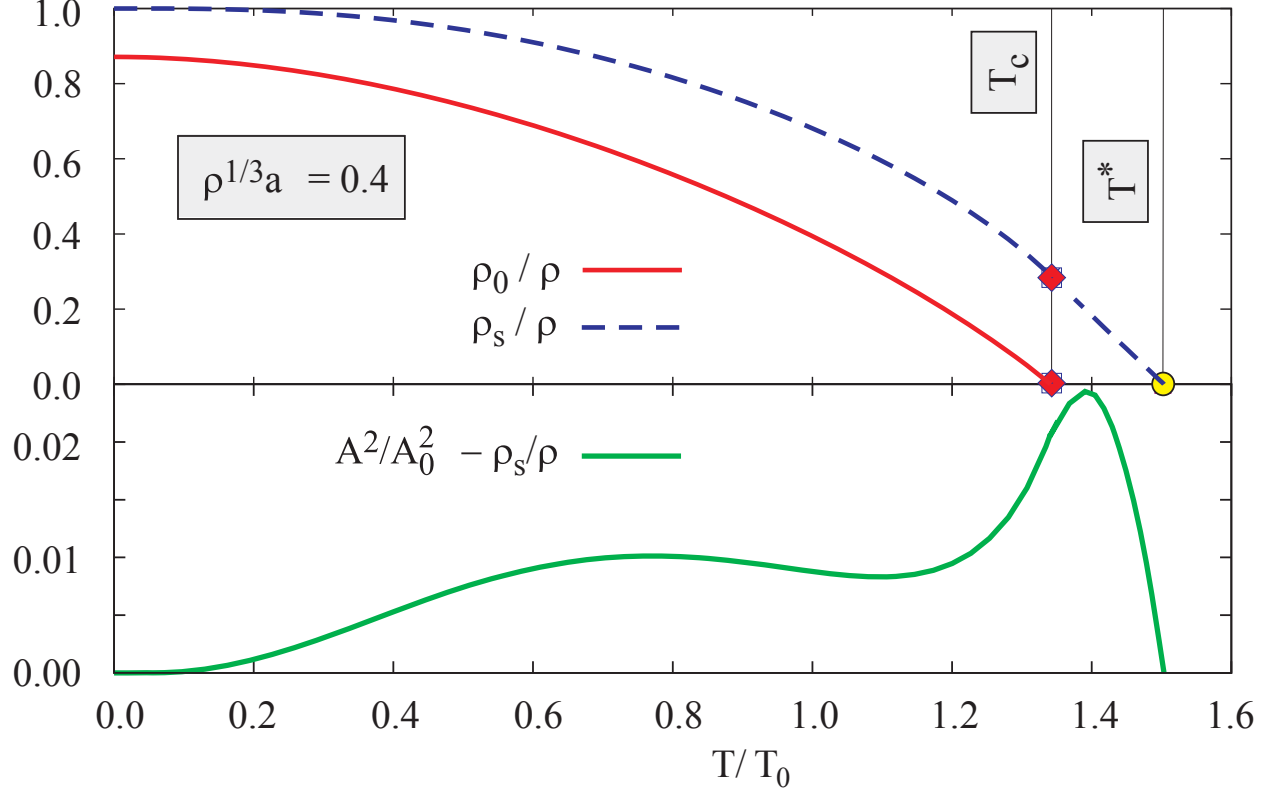


FIG. 9. (Color online) (top) Comparison of the atom BEC condensate density, ρ_0 , and the superfluid density, ρ_s , for $\rho^{1/3}a_0 = 0.4$. (bottom) Comparison of A^2 and ρ_s . Here $A_0 \equiv A(T = 0)$.

X. BOSE HUBBARD MODEL

This is the lattice version of the BEC problem, so we expand the inverse Green function in a three dimensional Fourier series,

$$\mathcal{G}_{\mathbf{i},\mathbf{j}}^{-1}(\tau, \tau') = \frac{1}{\beta N_s^3} \sum_{\mathbf{k}, n} \tilde{\mathcal{G}}_{\mathbf{k}, n}^{-1} e^{i[2\pi \mathbf{k} \cdot (\mathbf{i} - \mathbf{j}) / N_s - \omega_n (\tau - \tau')]} , \quad (81)$$

where $\omega_n = 2\pi n / \beta$ are the Bose Matsubara frequencies. Here $\mathbf{k} = (k_x, k_y, k_z)$ is a triplet of integers, each running from $-N_s/2$ to $N_s/2 - 1$. The total number of sites in the cubic box is N_s^3 and the *filling* factor, ν , is defined to be the number of particles per

site, $\nu = N/N_s^3$.

The Fourier transform of the Green function is again

$$\tilde{\mathcal{G}}_{\mathbf{k},n}^{-1} = \begin{pmatrix} \epsilon_{\mathbf{k}} + \chi' - i\omega_n & -A \\ -A^* & \epsilon_{\mathbf{k}} + \chi' + i\omega_n \end{pmatrix}, \quad (82)$$

where we have put $\chi' = \sqrt{2}\chi - \mu$. Now ϵ_k is given in terms of the lattice momentum, $\hat{\mathbf{k}}$, as

$$\epsilon_{\mathbf{k}} = J \hat{\mathbf{k}}^2 = 2J \sum_{s=x,y,z} [1 - \cos(2\pi k_s/N_s)], \quad (83)$$

The effective potential in LOAF is [5]

$$\begin{aligned} V_{\text{eff}}[\Phi, \Delta]/N_s^3 & \\ &= \chi' |\phi|^2 - \frac{1}{2} [A \phi^{*2} + A^* \phi^2] - \frac{(\chi' + \mu)^2}{4U} + \frac{|A|^2}{2U} \\ &+ \frac{1}{N_s^3} \sum_{\mathbf{k}} \left\{ \frac{1}{2} [\omega_k - \epsilon_k - \chi'] + \frac{1}{\beta} \ln[1 - e^{-\beta\omega_k}] \right\}. \end{aligned} \quad (84)$$

which leads to

$$(\chi' - A^*) \phi = 0, \quad (85a)$$

$$\frac{\chi' + \mu}{2U} = |\phi|^2 + \frac{1}{N_s^3} \sum_{\mathbf{k}} \left\{ \frac{\epsilon_k + \chi'}{2\omega_k} [2n_k + 1] - \frac{1}{2} \right\}, \quad (85b)$$

$$\frac{A}{U} = \phi^2 + \frac{A}{N_s^3} \sum_{\mathbf{k}} \frac{[2n_k + 1]}{2\omega_k}, \quad (85c)$$

where $n_k = 1/[e^{\beta\omega_k} - 1]$, $\omega_k = \sqrt{(\epsilon_k + \chi')^2 - |A|^2}$. and with the

filling factor given by

$$\nu = \frac{N}{N_s^3} = -\frac{1}{N_s^3} \frac{\partial V_{\text{eff}}[\Phi, \Delta]}{\partial \mu} = \frac{\chi' + \mu}{2U}. \quad (86)$$

We interpret $|\phi|^2$ as the number of condensed particles per site, and put

$$|\phi|^2 = \phi^2 = \nu_0 \frac{N_0}{N_s^3} = \nu n_0, \quad (87)$$

with the condensate fraction, $n_0 = N_0/N$. The sums over \mathbf{k} then omit the $\mathbf{k} = 0$ mode. The gap equations then become

$$\nu = \nu n_0 + \frac{1}{N_s^3} \sum_{\mathbf{k}}' \left\{ \frac{\epsilon_k + \chi'}{2\omega_k} [2n_k + 1] - \frac{1}{2} \right\}, \quad (88a)$$

$$\frac{A}{U} = \nu n_0 + \frac{A}{N_s^3} \sum_{\mathbf{k}}' \frac{[2n_k + 1]}{2\omega_k}, \quad (88b)$$

In obtaining our results we convert the finite sums over \mathbf{k} to integrals by defining $\mathbf{q} = 2\mathbf{k}/N_s$, so that formally we substitute

$$\frac{1}{N_s^3} \sum_{\mathbf{k}} \Rightarrow \iiint_{-1}^{+1} \frac{d^3 q}{8} = \iiint_0^{+1} d^3 q. \quad (89)$$

This substitution is exact in the limit $N_s \rightarrow \infty$.

The numerical analysis of the solutions space for Eqs. (88), leads to three distinct regions in the Bose-Hubbard model phase diagram:

I. The broken symmetry case where $\phi \neq 0$ and $\chi' = A$. Then

$\omega = \sqrt{\epsilon_k(\epsilon_k + 2\chi')}$. In this region, we solve the equations [22]:

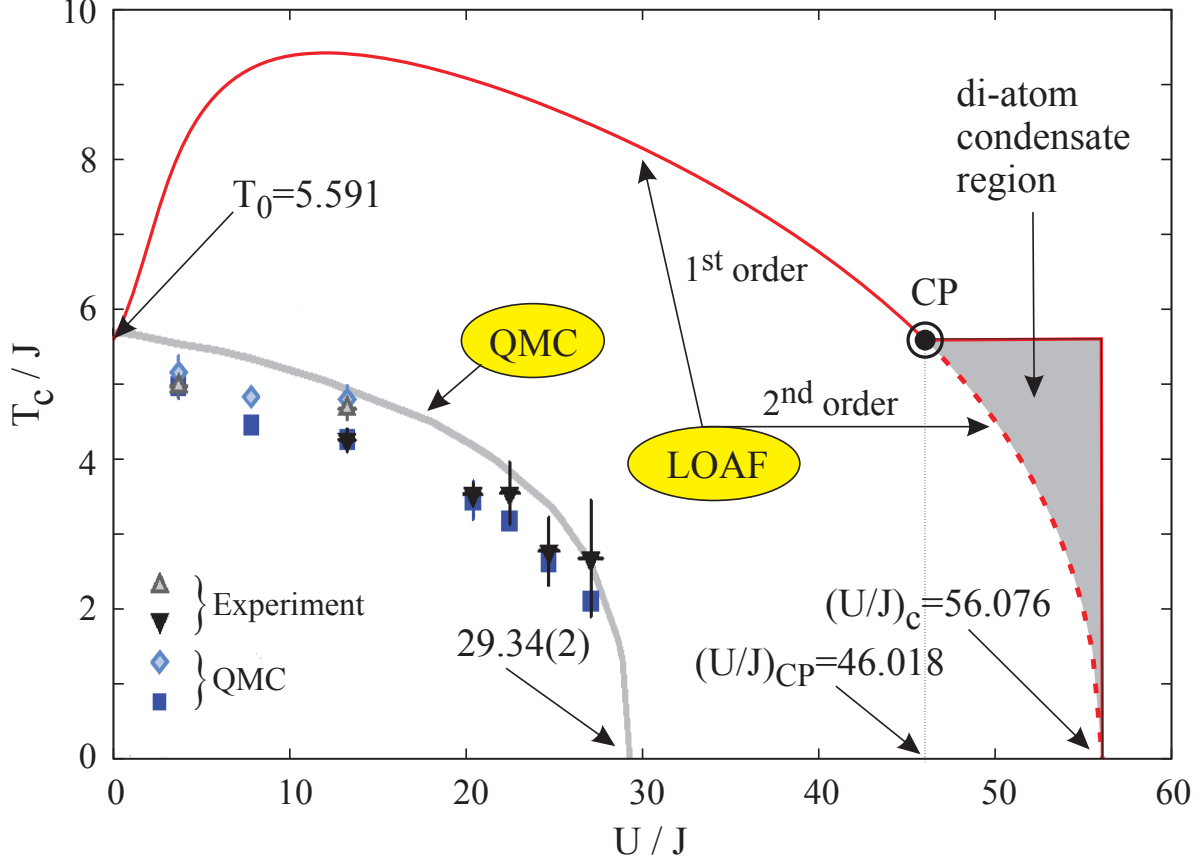


FIG. 10. (Color online) Comparison of the coupling constant dependence of the LOAF critical temperature, T_c , at unity filling, $\nu = 1$, with experimental [20] and quantum Monte Carlo (QMC) results [21]. The LOAF value of the critical Hubbard parameter value, $(U/J)_c = 56.076$, should be compared to the QMC critical value, $(U/J)_c = 29.34(2)$, reported in Ref. 21. LOAF also predicts a critical point at $(U/J)_{CP} = 46.02$. The solid and dashed lines indicate first- and second-order phase transitions predicted by LOAF theory, respectively. The shaded area depicts the region where a *diatom* condensate without the *usual* Bose-Einstein condensate is expected.

$$\nu = \nu n_0 + \frac{1}{N_s^3} \sum_{\mathbf{k}}' \left\{ \frac{\epsilon_k + \chi'}{2\omega_k} [2n_k + 1] - \frac{1}{2} \right\}, \quad (90a)$$

$$\frac{\chi'}{U} = \nu n_0 + \frac{\chi'}{N_s^3} \sum_{\mathbf{k}}' \frac{[2n_k + 1]}{2\omega_k}. \quad (90b)$$

II. The case when $\phi = 0$ so that $n_0 = 0$, and either

(i) $A = 0$ so that $\omega_k = \epsilon_k + \chi'$ and

$$\nu = \frac{1}{N_s^3} \sum_{\mathbf{k}}' n_k. \quad (91)$$

This solution corresponds to a first-order phase transition. Eq. (91) does not depend on the interaction strength and applies for temperatures, $T \geq T_c$, where T_c is the critical temperature defined by the zero condensate fraction limit, $n_0 \rightarrow 0$, in Eqs. (90).

(ii) or $0 \leq A \leq \chi'$ so that $\omega_k = \sqrt{(\epsilon_k + \chi')^2 - A^2}$, and

$$\nu = \frac{1}{N_s^3} \sum_{\mathbf{k}}' \left\{ \frac{\epsilon_k + \chi'}{2\omega_k} [2n_k + 1] - \frac{1}{2} \right\}, \quad (92a)$$

$$\frac{1}{U} = \frac{1}{N_s^3} \sum_{\mathbf{k}}' \frac{1}{2\omega_k} [2n_k + 1]. \quad (92b)$$

This solution corresponds to a second-order phase transition.

III. the normal case where $\phi = 0$ and $A = 0$. In this case we solve

Eq. (91) as in case II(i) above.

We note that the LOAF equations for the cubic lattice are identical with the LOAF equations for the continuum system [1, 2, 4].

ACKNOWLEDGMENTS

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