

Superfluidity without symmetry breaking: The time-dependent Hartree-Fock approximation for Bose-condensed condensates

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(Received 14 September 2005; published 21 August 2006)

We develop a time-dependent Hartree-Fock approximation that is appropriate for Bose-condensed systems. Defining a *depletion Green's function* allows the construction of condensate and depletion particle densities from eigenstates of a single time-dependent (oscillating) Hamiltonian, guaranteeing that our approach is a number-conserving approximation. The poles of this Green's function yield the energies of number-changing excitations for which the condensate particle number is held fixed, which we show has a gapped spectrum in the superfluid state. The linearized time-dependent version of this has poles at the collective frequencies of the system, yielding the expected zero sound mode for a uniform infinite system. We show how the approximations may be expressed in a general linear response formalism.

DOI: [10.1103/PhysRevA.74.023613](https://doi.org/10.1103/PhysRevA.74.023613)

PACS number(s): 03.75.Kk, 67.40.Db, 05.30.Jp

I. INTRODUCTION

The time-dependent Hartree-Fock approximation (TDHFA) is a powerful method for determining the properties of many-body systems [1]. It allows the computation of the density response functions, conductivities, and other linear response functions. The poles of such functions determine the collective modes of a system, and within the TDHFA the effects of thermally generated single particle excitations on these modes are included. The TDHFA has thus become a standard tool in condensed matter, nuclear, and atomic physics.

Surprisingly, the TDHFA has not enjoyed such success in the area of Bose-condensed systems [2]. In part this is because there are other powerful methods for computing collective modes, based on the Bogoliubov approximation in which there is coherence among states with different particle numbers; i.e., where gauge symmetry is spontaneously broken. Field theoretic techniques that incorporate this were developed long ago [3], but in light of the significant progress on atomic gases in the last decade [4], there is much renewed effort to improve upon these methods [5]. Among these are generalizations of various mean-field schemes to properly include the effects of symmetry breaking [6], and a “dielectric approach” that carefully treats Green's functions and response functions in a consistent way [7,8]. The challenge in these studies has been to treat the dynamics of the condensate and of the thermally excited (i.e., depleted) particles in a fully consistent manner. The resulting schemes are considerably more involved than the original Bogoliubov approach. (For a review, see Ref. [5].)

As we show below, one way to avoid the difficulties of disentangling the single-particle and collective excitations is to work with an ensemble in which the gauge symmetry is *not* broken [9]. In situations for which the particle number is relatively small, this may actually be preferable to broken symmetry approaches for which the associated fluctuations in the particle number can become problematic. Our chosen approach is the TDHFA. Its principle advantage is that the condensate wave function and the single-particle excitations appear as states of a *single* time-dependent, nonlocal Hamil-

tonian, so that they may be treated on an equal footing with exchange effects fully included. The connection through a single Hamiltonian guarantees that conservation laws will be respected [10], and we will demonstrate that the method correctly produces the gapless superfluid mode for a homogeneous system.

Our principal conclusions are as follows. (i) We find that in order to properly deal with exchange, one must adopt a *constrained* grand-canonical ensemble for the density matrix first introduced by Huse and Siggia [11], in which the number of particles in the condensate is fixed while the occupation probability for other single particle states is given by the standard grand-canonical ensemble. Within this ensemble, one finds a *gap* in the single-particle spectrum between the condensate and the other single-particle states [11,12], the latter of which we call depletion states [13]. This exchange gap is analogous to the single-particle gap that arises in superconducting systems and only arises when the system is Bose condensed, and thus may be viewed as a superfluid order parameter. The gap should be observable in a tunneling experiment between a normal Bose gas and a Bose condensate. (ii) We define a *depletion Green's function* $\tilde{G}(\mathbf{q}, \omega)$, whose poles occur at the single-particle energies of the depletion states in the Hartree-Fock (HF) approximation, which by construction does *not* have a pole at the collective mode frequency, as is expected for the full Green's function. The response of this Green's function to a weak, time-dependent perturbation, coupled with the equation of motion for the condensate wave function—which is a finite temperature generalization of the Gross-Pitaevskii (GP) equation—allows us to generate equations of motion for the condensate and depletion states governed by the *same* effective Hamiltonian, and to define response functions whose poles occur at the collective excitations of the system. This naturally captures the interplay between the condensate and depletion states. (iii) We solve these coupled equations for the simplest case of an infinite uniform Bose gas, and demonstrate that whenever there is Bose condensation, there is a gapless collective (zero sound) mode. This is usually identified as the superfluid mode in approaches where the gauge symmetry is broken; in our approach we find the mode even though the

symmetry is kept intact. We demonstrate that the density response function contains structure that could not arise in simple Bogoliubov approaches where only the collective mode is retained.

This paper is organized as follows: In Sec. II, we derive the static and time-dependent HF equations at finite temperature by using a constrained grand-canonical ensemble. We then show how this can be used to define the depletion Green's function which captures the energetics of particles outside the condensate. In Sec. III, we demonstrate how the depletion Green's function may be used to generate an approximate form for response functions. We also show that the same result may be obtained directly from wave functions, firmly establishing the connection with the TDFHA. In Sec. IV, we apply the general results in previous sections to a homogenous system with a contact two-body interaction. Discussions and conclusions are presented in the final section. Further details are presented in the Appendixes.

II. STATIC AND TIME-DEPENDENT HARTREE-FOCK EQUATIONS AT FINITE TEMPERATURE

We begin with Bose particles in an external potential $U(\vec{r})$ that is time independent. The Hamiltonian is

$$\hat{H} = \int d\vec{r} \hat{\psi}^\dagger(\vec{r}) H_0 \hat{\psi}(\vec{r}) + \frac{1}{2} \int d\vec{r}_1 d\vec{r}_2 \hat{\psi}^\dagger(\vec{r}_1) \hat{\psi}^\dagger(\vec{r}_2) \times V(\vec{r}_1 - \vec{r}_2) \hat{\psi}(\vec{r}_2) \hat{\psi}(\vec{r}_1), \quad (1)$$

where $H_0 = -\frac{\hbar^2 \nabla^2}{2m} + U(\vec{r})$ is the noninteracting Hamiltonian and $V(\vec{r}_1 - \vec{r}_2)$ the two-body potential. For a neutral Bose gas, V is usually short range and can be taken to have a contact form $V(\vec{r}) = g \delta(\vec{r})$ if the gas is dilute. We wish first to find the eigenstates of \hat{H} in the Hartree-Fock approximation (HFA) at finite temperature [11, 12].

We begin with the standard HFA, which we shall see is fine for high temperatures, but becomes a poor approximation when the system is Bose condensed. We seek a single-particle Hamiltonian

$$\hat{H}_{HF} = \sum_{\alpha\beta} \varepsilon_{\alpha\beta} a_\alpha^\dagger a_\beta, \quad (2)$$

where the indices α label states of a single-particle basis, which minimizes the free energy. In terms of these states the Hamiltonian Eq. (1) can be written

$$H = \sum_{\alpha\beta} \varepsilon_{\alpha\beta}^0 a_\alpha^\dagger a_\beta + \frac{1}{2} \sum_{\alpha\beta\delta\gamma} V_{\alpha\beta\delta\gamma} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma, \quad (3)$$

where

$$\varepsilon_{\alpha\beta}^0 = \int d\vec{r} \psi_\alpha^*(\vec{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + U(\vec{r}) \right] \psi_\beta(\vec{r}) \quad (4)$$

is the matrix element of the noninteracting Hamiltonian, with ψ_α the single particle states, and

$$V_{\alpha\beta\delta\gamma} = \int d\vec{r}_1 \int d\vec{r}_2 \psi_\alpha^*(\vec{r}_1) \psi_\beta^*(\vec{r}_2) V(\vec{r}_1 - \vec{r}_2) \psi_\delta(\vec{r}_2) \psi_\gamma(\vec{r}_1) \quad (5)$$

is the matrix element of the two-body potential.

At finite temperature $k_B T = 1/\beta$ where k_B is the Boltzmann constant, the expectation value of an operator \hat{O} is

$$\langle \hat{O} \rangle = \text{Tr} \hat{D} \hat{O}, \quad (6)$$

where \hat{D} is the exact density matrix operator. In the grand-canonical ensemble this is

$$\hat{D} = \frac{e^{-\beta(\hat{H} - \mu\hat{N})}}{\text{Tr} e^{-\beta(\hat{H} - \mu\hat{N})}} = \frac{1}{Z} e^{-\beta(\hat{H} - \mu\hat{N})}, \quad (7)$$

where Z is the corresponding partition function

$$Z = \text{Tr} e^{-\beta(\hat{H} - \mu\hat{N})}. \quad (8)$$

The Hartree-Fock approximation is based on the variational principle [1] that for any trial density matrix \hat{D}_r , one always has for the free energy

$$\Omega[\hat{D}_r] \geq \Omega[\hat{D}]. \quad (9)$$

In practice one chooses a form for \hat{D}_r that minimizes the free energy while allowing calculations with it to be tractable. In the Hartree-Fock approximation we choose trial density matrix

$$\hat{D}_{var} = \frac{1}{Z_{var}} e^{-\beta(\hat{H}_{HF} - \mu\hat{N})} \quad (10)$$

with

$$Z_{var} = \text{Tr} e^{-\beta(\hat{H}_{HF} - \mu\hat{N})}. \quad (11)$$

The parameters $\varepsilon_{\alpha\beta}$ and ψ_α are determined by minimizing the trial free energy [1]

$$\Omega_{var} = -\frac{1}{\beta} \ln Z_{var} - \text{Tr} \hat{D}_{var} \hat{H}_{HF} + \text{Tr} \hat{D}_{var} \hat{H}. \quad (12)$$

Defining the single-particle density matrix $\rho_{\alpha\beta}$ as

$$\rho_{\alpha\beta} = \text{Tr} \hat{D}_{var} a_\alpha^\dagger a_\beta, \quad (13)$$

one has

$$\text{Tr} \hat{D}_{var} \hat{H}_{HF} = \text{Tr} \rho \varepsilon. \quad (14)$$

The variation of Ω_{var} yields

$$\begin{aligned} \delta\Omega_{var} &= \frac{1}{Z_{var}} \text{Tr} e^{-\beta\hat{H}_{HF}} \delta\hat{H}_{HF} - \text{Tr} \delta\rho \varepsilon - \text{Tr} \rho \delta\varepsilon + \delta\langle \hat{H} \rangle \\ &= -\text{Tr} \varepsilon \delta\rho + \delta\langle \hat{H} \rangle = \text{Tr} \left(\frac{\delta\langle \hat{H} \rangle}{\delta\rho} - \varepsilon \right) \delta\rho, \end{aligned} \quad (15)$$

with

$$\langle \hat{H} \rangle = \sum_{\alpha\beta} \varepsilon_{\alpha\beta}^0 \rho_{\alpha\beta} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} [\rho_{\alpha\gamma} \rho_{\beta\delta} + \rho_{\alpha\delta} \rho_{\beta\gamma}]. \quad (16)$$

By requiring $\delta\Omega_{var}=0$, one arrives at

$$\varepsilon_{\alpha\beta} = \frac{\partial \langle \hat{H} \rangle}{\partial \rho_{\beta\alpha}} = \varepsilon_{\alpha\beta}^0 + \sum_{\gamma\delta} \bar{V}_{\alpha\gamma\beta\delta} \rho_{\delta\gamma}, \quad (17)$$

where $\bar{V}_{\alpha\gamma\beta\delta} = V_{\alpha\gamma\beta\delta} + V_{\alpha\gamma\delta\beta}$. This is the Hartree-Fock equation in an arbitrary single-particle basis.

A. Constrained grand-canonical ensemble

The above derivation is valid for all temperatures, and the condensate plays no special role. However, the result has significant problems for a Bose-condensed system: (i) It predicts macroscopically large fluctuations in the total particle number of the system below the critical temperature, which is unphysical. In the diagonal basis where $n_\alpha = \rho_{\alpha\alpha} = (e^{\beta(\varepsilon_\alpha - \mu)})^{-1}$, the source of this problem may be traced to the parameter $\varepsilon_{\alpha=0} - \mu$ associated with the condensate wave function, which becomes arbitrarily small in the thermodynamic limit [14]. (ii) With a contact interaction, the grand-canonical ensemble produces the same mean-field potential for all particles, and does not yield the expected appearance of an exchange energy only when particles are in different states, not when they are in the same state. This is not a serious problem when the system is above the critical temperature since each level is microscopically occupied. However, this is a poor approximation when the system is Bose condensed.

To correct these problems, one may introduce a *constrained* trial grand canonical ensemble [11]

$$D'_{var} = \frac{1}{Z'_{var}} \text{Tr} e^{-\beta \sum_\alpha (\varepsilon_\alpha - \mu) a_\alpha^\dagger a_\alpha} \delta_{a_0^\dagger a_0, N_0}. \quad (18)$$

with Z'_{var} chosen as usual to normalize the distribution. In this expression we have expressed \hat{H}_{HF} in a diagonal basis. As we shall see below, the wave functions associated with the operators are determined by minimizing the free energy within this trial ensemble. The resulting condensate wave function created by a_0^\dagger turns out to have the lowest eigenvalue of an effective Hamiltonian, and so becomes the eigenstate of the single-body density operator with the largest eigenvalue [9].

This ensemble essentially excludes the *dangerous* condensed mode from statistical averaging [15], since this is what causes the problem in standard HF. As we will see, this removes the spurious exchange energy among particles occupying the condensate mode, while keeping it among particles occupying different levels. Consistent treatment of exchange in a Bose condensed system turns out to be essential for obtaining the expected gapless superfluid mode of an infinite uniform system.

Using Eq. (18), one gets the variational free energy

$$\Omega_{var} = -\mu N_0 + \sum_{\alpha \neq 0} [k_B T \ln(n_\alpha + 1) - \varepsilon_\alpha n_\alpha] + \langle \hat{H} \rangle, \quad (19)$$

where $\langle \hat{H} \rangle$ is

$$\langle \hat{H} \rangle = \sum_{\alpha} \varepsilon_{\alpha\alpha}^0 n_\alpha + \frac{1}{2} \sum_{\alpha\beta} \bar{V}_{\alpha\beta\alpha\beta} n_\alpha n_\beta - \frac{1}{2} V_{0000} N_0^2 \quad (20)$$

and

$$n_\alpha = N_0 \delta_{\alpha,0} + \frac{1}{e^{-\beta(\varepsilon_\alpha - \mu)} - 1} \delta_{\alpha \neq 0}. \quad (21)$$

When Ω_{var} is minimized with respect to N_0 and n_α ($\alpha \neq 0$), which is equivalent to variation with respect to ε_α , one finds

$$0 = -\mu + \frac{\partial \langle \hat{H} \rangle}{\partial N_0}, \quad \alpha = 0, \quad (22)$$

$$0 = \frac{\partial \ln(n_\alpha + 1)}{\partial n_\alpha} - \varepsilon_\alpha - n_\alpha \frac{\partial \varepsilon_\alpha}{\partial n_\alpha} + \frac{\partial \langle \hat{H} \rangle}{\partial n_\alpha}, \quad \alpha \neq 0. \quad (23)$$

These equations are straightforwardly solved by setting

$$\begin{aligned} \varepsilon_\alpha &= \varepsilon_{\alpha\alpha}^0 + \sum_{\beta} [V_{\alpha\beta\alpha\beta} + V_{\alpha\beta\beta\alpha}] n_\beta - V_{0000} N_0 \delta_{\alpha,0} \\ &= \varepsilon_{\alpha\alpha}^0 + \Sigma_{\alpha\alpha}, \quad \text{for all } \alpha \end{aligned} \quad (24)$$

and

$$\mu = \varepsilon_0, \quad (25)$$

where

$$\Sigma_{\alpha\alpha} = \sum_{\beta} [V_{\alpha\beta\alpha\beta} + V_{\alpha\beta\beta\alpha}] n_\beta - V_{0000} N_0 \delta_{\alpha,0} \quad (26)$$

is the diagonal matrix element of the Hartree-Fock self-energy.

The problem is not fully solved because we do not have expressions for the wave functions that determine the matrix elements $V_{\alpha\beta\gamma\delta}$. To find these, we minimize the free energy with respect to the single-particle wave functions, keeping in mind that they must form a complete orthonormal set [11]. This constraint may be enforced if we write the variation in the form

$$\delta\psi_\alpha = \sum_{\gamma} \eta_{\alpha\gamma} \psi_\gamma, \quad \text{or} \quad \delta a_\alpha^\dagger = \sum_{\gamma} \eta_{\alpha\gamma} a_\gamma^\dagger, \quad (27)$$

where $\eta_{\beta\alpha} = -\eta_{\alpha\beta}^*$. The resulting variation of the free energy Ω_{var} may be written

$$\delta\Omega_{var} = \sum_{\mu \neq \nu} \eta_{\nu\mu} \langle [H, a_\mu^\dagger a_\nu] \rangle. \quad (28)$$

The proof of this result is given in Appendix A, and is valid whether or not the system is Bose condensed. The expectation value is calculated with respect to the constrained ensemble. Now substituting Eq. (3) into Eq. (28), one gets

$$\begin{aligned} \delta\Omega_{var} = & \sum_{\mu \neq \nu} \eta_{\nu\mu} \left[\varepsilon_{\nu\mu}^0 + \sum_{\gamma} \bar{V}_{\nu\gamma\gamma\mu} n_{\gamma} - V_{\nu\nu\mu} n_{\nu} \delta_{\nu,0} \right] n_{\nu} \\ & + \sum_{\mu \neq \nu} \eta_{\mu\nu}^* \left[\varepsilon_{\nu\mu}^0 + \sum_{\gamma} \bar{V}_{\nu\gamma\gamma\mu} n_{\gamma} - V_{\nu\mu\mu} n_{\mu} \delta_{\mu,0} \right] n_{\mu}. \end{aligned} \quad (29)$$

The free energy should be stationary with respect to variations in η ,

$$\frac{\delta\Omega_{var}}{\delta\eta_{\nu\mu}} = \frac{\delta\Omega_{var}}{\delta\eta_{\mu\nu}^*} = 0, \quad (30)$$

which results in the equation

$$\varepsilon_{\nu\mu}^0 + \sum_{\gamma} \bar{V}_{\nu\gamma\gamma\mu} n_{\gamma} - N_0(V_{\nu\mu\mu} \delta_{\mu,0} + V_{\nu\nu\mu} \delta_{\nu,0}) = 0. \quad (31)$$

Equation (31) suggests that the self-energy matrix should be defined as follows [11]:

$$\begin{aligned} \Sigma_{\nu\mu} = & \sum_{\gamma} \bar{V}_{\nu\gamma\gamma\mu} n_{\gamma} - N_0(V_{\nu\mu\mu} \delta_{\mu,0} + V_{\nu\nu\mu} \delta_{\nu,0}) \\ & + N_0 V_{0000} \delta_{\nu,0} \delta_{\mu,0}, \end{aligned} \quad (32)$$

which we note is consistent with our earlier definition of the diagonal self-energy matrix elements. In real space this may be written

$$\begin{aligned} \Sigma(\vec{r}_1, \vec{r}_2) = & \sum_{\nu\mu} \Sigma_{\nu\mu} \psi_{\nu}(\vec{r}_1) \psi_{\mu}^*(\vec{r}_2) \\ = & \delta(\vec{r}_1 - \vec{r}_2) \int d\vec{r}_3 V(\vec{r}_2 - \vec{r}_3) \rho(\vec{r}_3, \vec{r}_3) \\ & + V(\vec{r}_1 - \vec{r}_2) \rho(\vec{r}_1, \vec{r}_2) \\ & - N_0 \int d\vec{r}_3 W_0(\vec{r}_3, \vec{r}_3) [V(\vec{r}_1 - \vec{r}_3) \\ & + V(\vec{r}_2 - \vec{r}_3)] W_0(\vec{r}_1, \vec{r}_2) + N_0 V_{0000} W_0(\vec{r}_1, \vec{r}_2) \end{aligned} \quad (33)$$

where $\rho(\vec{r}_1, \vec{r}_2)$ is

$$\rho(\vec{r}_1, \vec{r}_2) = \sum_{\alpha} n_{\alpha} \psi_{\alpha}(\vec{r}_1) \psi_{\alpha}^*(\vec{r}_2), \quad (34)$$

and $W_{\alpha}(\vec{r}_1, \vec{r}_2)$ is defined

$$W_{\alpha}(\vec{r}_1, \vec{r}_2) = \psi_{\alpha}(\vec{r}_1) \psi_{\alpha}^*(\vec{r}_2). \quad (35)$$

With these definitions, and using the completeness of the basis, Eq. (31) is equivalent to the Hartree-Fock equation

$$\left[-\frac{\nabla^2}{2m} + U(\vec{r}) \right] \psi_{\alpha}(\vec{r}) + \int d\vec{r}' \Sigma(\vec{r}, \vec{r}') \psi_{\alpha}(\vec{r}') = \varepsilon_{\alpha} \psi_{\alpha}(\vec{r}) \quad (36)$$

with

$$\varepsilon_{\alpha} = \varepsilon_{\alpha\alpha}^0 + \sum_{\beta} \bar{V}_{\alpha\beta\beta\alpha} n_{\beta} - N_0 V_{0000} \delta_{\alpha,0}. \quad (37)$$

The form of the self-energy in Eq. (33), as most clearly expressed in Eq. (32), has an interesting consequence: the

self-energy for the bosons in the condensate is different than that of higher energy states. For the case of a uniform, infinite system this means there is a gap between the single-particle energy of the condensate and those of the excited states. This property of Bose condensates is well-known [16], and finding an appropriate way to deal with it is one of the major challenges in developing approximations for the excitation spectrum of a Bose-Einstein condensate (BEC) [5]. For the case of a uniform infinite system, this gap is present in the single-particle spectrum in spite of the expected gapless collective mode spectrum. In order to deal with this, it is helpful to develop different Green's functions which capture one or the other portion of the excitation spectrum, as we now proceed to do.

B. Depletion Green's function and the TDHFA

In formulating a TDHFA, it is useful to define Green's functions in imaginary time and consider self-consistent approximations to their equations of motion [10]. In the fermion case, poles of the Green's function in the absence of a time-dependent potential gives the spectrum of number-changing excitations, while the response of these Green's functions to time-dependent potentials give collective excitations. This allows one to conveniently separate out these sectors of the energy spectrum. In a Bose condensed state, these sectors become entangled in the standard Green's function because one may add a particle to the condensate and then excite a collective mode, yielding poles at collective mode frequencies. Disentangling the single-particle spectrum from the collective mode spectrum in the Green's function then becomes quite challenging.

As we now demonstrate, the TDHFA for Bose condensates can be developed in a way that is analogous to what works so well for fermion systems. To this we define a *depletion Green's function*, incorporating all the information about the single-particle states other than that of the condensate. Within the static Hartree-Fock approximation this has the form

$$\tilde{G}(\vec{r}_1, \vec{r}_2; i\omega_n) = \sum_{\alpha \neq 0} \frac{\psi_{\alpha}(\vec{r}_1) \psi_{\alpha}^*(\vec{r}_2)}{i\omega_n - \varepsilon_{\alpha} + \mu}. \quad (38)$$

Writing this Green's function in imaginary time, $\tilde{G}(\mathbf{r}_1 \tau_1, \mathbf{r}_2 \tau_2) = \frac{1}{\beta} \sum_n e^{-i\omega_n(\tau_1 - \tau_2)} \tilde{G}(\mathbf{r}_1, \mathbf{r}_2; i\omega_n)$ one may easily show that it satisfies the equation of motion

$$\begin{aligned} \left[-\frac{\partial}{\partial \tau_1} - H_0(\vec{r}_1) \right] \tilde{G}(\vec{r}_1 \tau_1, \vec{r}_2 \tau_2) - \int d\vec{r} \Sigma(\vec{r}_1, \vec{r}) \tilde{G}(\vec{r} \tau_1, \vec{r}_2 \tau_2) \\ = \delta(\tau_1 - \tau_2) [\delta(\vec{r}_1 - \vec{r}_2) - \psi_0(\vec{r}_1) \psi_0^*(\vec{r}_2)]. \end{aligned} \quad (39)$$

By excluding the condensate state from the depletion Green's function, we avoid the process that leads to poles at the collective mode frequencies. The lowest energy poles then reflect the single-particle spectrum.

To compute collective modes of the system, it is convenient to look at Green's functions in the presence of a time-dependent potential [10]. The natural generalization of Eq. (39) to this situation is

$$\left[-\frac{\partial}{\partial \tau_1} - H_0(\vec{r}_1) - \delta U(\vec{r}_1, \tau_1) \right] \tilde{G}(\vec{r}_1 \tau_1, \vec{r}_2 \tau_2) - \int d\vec{r} \int d\tau \Sigma(\vec{r}_1 \tau_1, \vec{r} \tau) \tilde{G}(\vec{r} \tau, \vec{r}_2 \tau_2) = \delta(\tau_1 - \tau_2) [\delta(\vec{r}_1 - \vec{r}_2) - \psi_0(\vec{r}_1, \tau_1) \psi_0^*(\vec{r}_2, \tau_2)], \quad (40)$$

where δU is a time-dependent potential which we will ultimately treat perturbatively. Note that in writing down this equation, the self-energy Eq. (33) now has time dependence, and is explicitly given by

$$\Sigma(\vec{r}_1 \tau_1, \vec{r}_2 \tau_2; \delta U) = \delta(\tau_1 - \tau_2) \left[\delta(\vec{r}_1 - \vec{r}_2) \int d\vec{r}_3 V(\vec{r}_2 - \vec{r}_3) \rho(\vec{r}_3 \tau_1, \vec{r}_3 \tau_1; \delta U) + V(\vec{r}_1 - \vec{r}_2) \rho(\vec{r}_1 \tau_1, \vec{r}_2 \tau_1; \delta U) \right] - \delta(\tau_1 - \tau_2) N_0 \left\{ \int d\vec{r}_3 [V(\vec{r}_1 - \vec{r}_3) + V(\vec{r}_2 - \vec{r}_3)] W_0(\vec{r}_3 \tau_1, \vec{r}_3 \tau_1; \delta U) - V_{0000} \right\} W_0(\vec{r}_1 \tau_1, \vec{r}_2 \tau_1; \delta U). \quad (41)$$

The time dependence enters through the *wave functions* in the quantities ρ and W_α [Eqs. (34) and (35)], and we have noted that these quantities are now functionals of δU which is ultimately responsible for the time dependence.

It is useful to note at this point that we have made a crucial assumption, which can be understood as the essential underlying approximation of the TDHFA: we allow only the wave functions to change with time, while the occupations n_α remain stationary and equal to their values for $\delta U=0$. This can be shown [1] to be equivalent to an assumption that the entropy of the system remains unchanged in the presence of δU . We note, however, that this is not equivalent to the statement that the system does not absorb energy from a time-dependent potential, because the (time-averaged) energies of the single-particle states are generally increased by the perturbation.

Noting that Eq. (34) may be recast in the form

$$\rho(\vec{r}_1 \tau_1, \vec{r}_2 \tau_2) = [\tilde{G}(\vec{r}_2, \tau_1^+, \vec{r}_1, \tau_1) + N_0 W_0(\vec{r}_1 \tau_1, \vec{r}_2 \tau_1)] \delta(\tau_1 - \tau_2), \quad (42)$$

with $W_0(\vec{r}_1 \tau_1, \vec{r}_2 \tau_1) = \psi_0(\vec{r}_1 \tau_1) \psi_0^*(\vec{r}_2 \tau_2)$, we see that Eqs. (33), (40), and (42) nearly form a closed set of equations. We have left to determine the time dependence of ψ_0 . An important aspect of the problem is to assure that our TDHFA obeys particle conservation, a feature that is often difficult to build into collective mode calculations for Bose condensates [5]. This is due to the fact that the condensate and depletion particles must be treated in different ways, so that often the total density and total current do not obey the continuity equation in their response to a time-dependent potential. In the present case, by contrast, we are guaranteed that the continuity equation will be obeyed because the condensate wave function is controlled by the same effective Hamiltonian as the excited states, via Eq. (40). Thus we take

$$\left[-\frac{\partial}{\partial \tau_1} - H_0(\vec{r}_1) - \delta U(\vec{r}_1, \tau_1) \right] \psi_0(\vec{r}_1 \tau_1) - \int d\vec{r} \int d\tau \Sigma(\vec{r}_1 \tau_1, \vec{r} \tau) \psi_0(\vec{r} \tau) = 0. \quad (43)$$

With this equation for ψ_0 , it is easy to verify that the overlaps

$\int d\mathbf{r} \psi_0^*(\mathbf{r} \tau) \tilde{G}(\mathbf{r} \tau, \mathbf{r}' \tau')$ and $\int d\mathbf{r}' \tilde{G}(\mathbf{r} \tau, \mathbf{r}' \tau') \psi_0(\mathbf{r}' \tau')$ vanish, so that the depletion Green's function involves no change in the number of condensate particles even in the presence of the time-dependent potential. It is the possibility of changing this and simultaneously creating a collective excitation that allows the collective mode spectrum to appear in the standard Green's function. Thus by working with the depletion Green's function we avoid the entangling of particle-conserving excitations and single-particle excited states that characterize the approaches based on broken gauge symmetry.

In principle these equations may be solved self-consistently to develop a mean-field approximation for this many-body system in a time-dependent potential. In practice this is a formidable task, so one instead focuses on the linear response of \tilde{G} and ψ_0 to small perturbations δU . These may be used to construct, for example, the density response function, whose poles give the collective modes of the system [10].

III. LINEAR RESPONSE

A. General formulation

We begin by expanding Eq. (40) for small δU , retaining only terms that are linear in this quantity. This leads to the equation

$$\begin{aligned} & \delta U(\vec{r}_1 \tau_1) \bar{W}_0(\vec{r}_1, \vec{r}_2) \delta(\tau_1 - \tau_2) \\ &= \left[\frac{\partial}{\partial \tau_2} - \hat{H}_{HF}(\vec{r}_2) \right] \delta(\tau_1 - \tau_2) \delta W_0(\vec{r}_1, \vec{r}_2; \tau_1) \\ &+ \left[-\frac{\partial}{\partial \tau_1} - \hat{H}_{HF}(\vec{r}_1) \right] \left[\frac{\partial}{\partial \tau_2} - \hat{H}_{HF}(\vec{r}_2) \right] \delta \tilde{G}(\vec{r}_1, \tau_1; \vec{r}_2, \tau_2) \\ &- \int d\vec{r}_3 \delta \Sigma(\vec{r}_1 \tau_1; \vec{r}_2 \tau_2) \bar{W}_0(\vec{r}_3, \vec{r}_2) \delta(\tau_1 - \tau_2), \end{aligned} \quad (44)$$

where $\bar{W}_0(\vec{r}_1, \vec{r}_2) = \delta(\vec{r}_1 - \vec{r}_2) - W_0(\vec{r}_1, \vec{r}_2)$, and $\delta W_0(\vec{r}_1, \vec{r}_2; \tau) = \delta \psi_0(\vec{r}_1, \tau) \psi_0^*(\vec{r}_2) + \psi_0(\vec{r}_1) \delta \psi_0^*(\vec{r}_2, \tau)$. The operator $\hat{H}_{HF}(\vec{r})$ has the meaning, for example,

$$\hat{H}_{HF}(\vec{r}_2) \delta W_0(\vec{r}_1, \vec{r}_2; \tau_1) = H_0(\vec{r}_2) \delta W_0(\vec{r}_1, \vec{r}_2; \tau_1) + \int d\vec{r} \Sigma(\vec{r}_2, \vec{r}) \delta W_0(\vec{r}_1, \vec{r}; \tau_1)$$

with Σ given by Eq. (33). The variation of the self-energy, $\delta\Sigma$, comes from the fact that the wave functions ψ_α are functionals of δU ; we will provide an explicit expression for the specific case of a contact potential below. Before proceeding with this, we demonstrate that the ideas developed above may be used to compute an important quantity, the density response function.

B. Density response function

An alternative procedure for avoiding the singularity in the standard imaginary time Green's function is to work directly with the wave functions and the density matrix

$$\rho(\vec{r}_1, \vec{r}_2, \tau; \delta U) = \sum_\alpha n_\alpha \psi_\alpha(\vec{r}_1, \tau) \psi_\alpha^*(\vec{r}_2, \tau),$$

which is a generalization of Eq. (34). In this context it is convenient to work with real rather than imaginary time. The equation of motion for a real time density matrix $\rho(\vec{r}_1, \vec{r}_2, t; \delta U)$ can be easily obtained from the time-dependent Hartree-Fock equations for the wave functions,

$$i \frac{\partial}{\partial t_1} \psi_\alpha(\vec{r}_1 t_1) = \left[-\frac{\nabla_1^2}{2m} + U(\vec{r}_1) + \delta U(\vec{r}_1 t_1) \right] \psi_\alpha(\vec{r}_1 t_1) + \int d\vec{r}_2 dt_2 \Sigma(\vec{r}_1 t_1, \vec{r}_2 t_2; \delta U) \psi_\alpha(\vec{r}_2 t_2), \quad (45)$$

with the result

$$0 = \left[i \frac{\partial}{\partial t} + \left(\frac{\nabla_1^2}{2m} - \frac{\nabla_2^2}{2m} \right) - U(\vec{r}_1 t) + U(\vec{r}_2 t) \right] \rho(\vec{r}_1, \vec{r}_2, t; \delta U) - \int d\vec{r}_3 [\Sigma(\vec{r}_1 t, \vec{r}_3 t; \delta U) \rho(\vec{r}_3, \vec{r}_2, t; \delta U) - \rho(\vec{r}_1, \vec{r}_3, t; \delta U) \Sigma(\vec{r}_3 t, \vec{r}_2 t; \delta U)]. \quad (46)$$

In writing this equation we have analytically continued the

self-energy to real time, which in practice simply involves replacing $\tau \rightarrow t$ in all the arguments of Eq. (41).

Expanding $\rho(\vec{r}_1, \vec{r}_2, t; \delta U)$, $\Sigma(\vec{r}_1 t, \vec{r}_2 t; \delta U)$, and $W_0(\vec{r}_1 t, \vec{r}_2 t; \delta U)$ around their static HF values and retaining only terms that are first order in $\delta U(\vec{r}t)$, one obtains a linearized equation for $\delta\rho$,

$$\begin{aligned} & [\delta U(\vec{r}_1 t) - \delta U(\vec{r}_2 t)] \rho(\vec{r}_1, \vec{r}_2) \\ &= \left[i \frac{\partial}{\partial t} - \hat{H}_{HF}(\vec{r}_1) + \hat{H}_{HF}(\vec{r}_2) \right] \delta \rho(\vec{r}_1 t, \vec{r}_2 t^+; U) \\ &\quad - \int d\vec{r}_3 [\delta \Sigma(\vec{r}_1 t, \vec{r}_3 t; \delta U) \rho(\vec{r}_3, \vec{r}_2) \\ &\quad - \rho(\vec{r}_1, \vec{r}_3) \delta \Sigma(\vec{r}_3 t, \vec{r}_2 t; \delta U)]. \end{aligned} \quad (47)$$

A density matrix response function [10] may be defined as follows:

$$\chi^R(\vec{r}_1 \vec{r}_3, \vec{r}_2 \vec{r}_3, t - t_3) = \theta(t - t_3) \left. \frac{\delta \rho(\vec{r}_1, \vec{r}_2, t; \delta U)}{\delta U(\vec{r}_3 t_3)} \right|_{\delta U=0}, \quad (48)$$

with the more standard density-density response function then given by $\chi^R(\vec{r}_1 \vec{r}_3, \vec{r}_1 \vec{r}_3, t - t_3)$. One can rewrite Eq. (47) as follows:

$$\begin{aligned} & \left[i \frac{\partial}{\partial t} - \hat{H}_{HF}(\vec{r}_1) + \hat{H}_{HF}(\vec{r}_2) \right] \chi^R(\vec{r}_1 \vec{r}_4, \vec{r}_2 \vec{r}_4, t - t_4) \\ &= [\delta(\vec{r}_1 - \vec{r}_4) - \delta(\vec{r}_2 - \vec{r}_4)] \delta(t - t_4) \rho(\vec{r}_1, \vec{r}_2) \\ &\quad + \int d\vec{r}_3 [\Gamma^R(\vec{r}_1 \vec{r}_4, \vec{r}_3 \vec{r}_4, t - t_4) \rho(\vec{r}_3, \vec{r}_2) \\ &\quad - \rho(\vec{r}_1, \vec{r}_3) \Gamma^R(\vec{r}_3 \vec{r}_4, \vec{r}_2, \vec{r}_4, t - t_4)], \end{aligned} \quad (49)$$

where

$$\begin{aligned} \Gamma^R(\vec{r}_1 \vec{r}_4, \vec{r}_2 \vec{r}_4, t - t_4) &= \theta(t - t_4) \left. \frac{\delta \Sigma(\vec{r}_1 t, \vec{r}_2 t; \delta U)}{\delta U(\vec{r}_4 t_4)} \right|_{\delta U=0} \\ &= \delta(\vec{r}_1 - \vec{r}_2) \int d\vec{r}_3 V(\vec{r}_2 - \vec{r}_3) \chi^R(\vec{r}_3 \vec{r}_4, \vec{r}_3 \vec{r}_4, t - t_4) + V(\vec{r}_1 - \vec{r}_2) \chi^R(\vec{r}_1 \vec{r}_4, \vec{r}_2 \vec{r}_4, t - t_4) \\ &\quad - N_0 \int d\vec{r}_3 [V(\vec{r}_1 - \vec{r}_3) + V(\vec{r}_2 - \vec{r}_3)] \left. \frac{\delta W_0(\vec{r}_3 t, \vec{r}_3 t; \delta U)}{\delta U(\vec{r}_4 t_4)} \right|_{\delta U=0} W_0(\vec{r}_1, \vec{r}_2) \\ &\quad - N_0 \left\{ \int d\vec{r}_3 [V(\vec{r}_1 - \vec{r}_3) + V(\vec{r}_2 - \vec{r}_3)] W_0(\vec{r}_3, \vec{r}_3) - V_{0000} \right\} \left. \frac{\delta W_0(\vec{r}_1 t, \vec{r}_2 t; \delta U)}{\delta U(\vec{r}_4 t_4)} \right|_{\delta U=0} \\ &\quad + 2N_0 \int d\vec{r}_3 \int d\vec{r}_5 V(\vec{r}_3 - \vec{r}_5) \left. \frac{\delta W_0(\vec{r}_3 t, \vec{r}_3 t; \delta U)}{\delta U(\vec{r}_4 t_4)} \right|_{\delta U=0} W_0(\vec{r}_5, \vec{r}_5) W_0(\vec{r}_1, \vec{r}_2). \end{aligned} \quad (50)$$

The functional derivative of W_0 with respect to $\delta U(\vec{r}t)$ requires one to work directly with the wave functions. This is discussed in detail in Appendix B, with the result [Eq. (B10)]

$$\begin{aligned} & \left. \frac{\delta W_0(\vec{r}_1 t_1, \vec{r}'_1 t_1; \delta U)}{\delta U(\vec{r}_2 t_2)} \right|_{\delta U=0} \\ &= - \sum_{\beta\lambda\mu} \int \frac{d\omega}{2\pi} \frac{e^{-i\omega(t_1-t_2)}}{\omega + \varepsilon_\beta - \varepsilon_0} [\delta_{0\lambda} \delta_{\beta\mu} + \Gamma_{0\beta,\lambda\mu}^R(\omega)] \\ & \quad \times \psi_\lambda^*(\vec{r}_2) \psi_\mu(\vec{r}_2) \psi_0(\vec{r}_1) \psi_\beta^*(\vec{r}'_1) \\ & \quad + \sum_{\beta\lambda\mu} \int \frac{d\omega}{2\pi} \frac{e^{-i\omega(t_1-t_2)}}{\omega + \varepsilon_0 - \varepsilon_\beta} [\delta_{0\mu} \delta_{\beta\lambda} + \Gamma_{\beta 0,\lambda\mu}^R(\omega)] \\ & \quad \times \psi_\lambda^*(\vec{r}_2) \psi_\mu(\vec{r}_2) \psi_\beta(\vec{r}_1) \psi_0^*(\vec{r}'_1). \end{aligned} \quad (51)$$

To make further progress, it is convenient to expand the functions χ^R and Γ^R in terms of the static HF eigenstates ψ_α as follows:

$$\begin{aligned} & \chi^R(\vec{r}_1 \vec{r}_3, \vec{r}_2 \vec{r}_3, t - t_3) \\ &= \sum_{\alpha\beta} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \chi_{\alpha\beta,\lambda\mu}(\omega) e^{-i\omega(t-t_3)} \psi_\beta^*(\vec{r}_2) \psi_\alpha(\vec{r}_1) \psi_\mu^*(\vec{r}_3) \psi_\lambda(\vec{r}_3), \\ & \Gamma^R(\vec{r}_1 \vec{r}_3; \vec{r}_2 \vec{r}_3, t_1 - t_3) \\ &= \sum_{\alpha\beta} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \psi_\alpha^*(\vec{r}_2) \psi_\beta(\vec{r}_1) \psi_\lambda^*(\vec{r}_3) \psi_\mu(\vec{r}_3) \Gamma_{\beta\alpha,\lambda\mu}^R(\omega) e^{-i\omega(t_1-t_3)}. \end{aligned} \quad (52)$$

Substituting these expansions into Eqs. (49)–(51), one obtains

$$(\omega + \varepsilon_\mu - \varepsilon_\lambda) \chi_{\lambda\mu,\alpha\beta}^R(\omega) = (n_\mu - n_\lambda) [\delta_{\lambda\alpha} \delta_{\mu\beta} + \Gamma_{\lambda\mu,\alpha\beta}^R(\omega)], \quad (53)$$

and

$$\begin{aligned} \Gamma_{\lambda\mu,\alpha\beta}^R(\omega) &= \sum_{\lambda_1\mu_1} [V_{\lambda\mu_1\lambda_1\mu} + V_{\lambda\mu_1\mu\lambda_1}] \chi_{\lambda_1\mu_1,\alpha\beta}^R(\omega) - \sum_{\lambda_1\mu_1} \delta_{\lambda_1 0} [V_{\lambda\mu_1\mu\lambda_1} \delta_{\lambda_1\mu} + V_{\lambda\mu_1\lambda_1\mu} \delta_{\lambda_1\lambda}] \chi_{\lambda_1\mu_1,\alpha\beta}^R(\omega) - \sum_{\lambda_1\mu_1} \delta_{\mu_1 0} [V_{\lambda\mu_1\lambda_1\mu} \delta_{\mu_1\mu} \\ & \quad + V_{\lambda\mu_1\mu\lambda_1} \delta_{\mu_1\lambda}] \chi_{\lambda_1\mu_1,\alpha\beta}^R(\omega) - \sum_{\lambda_1\mu_1} (\delta_{\lambda_1 0} + \delta_{\mu_1 0}) (\delta_{\lambda_1\lambda} V_{\mu_1 0\mu} + \delta_{\mu_1\mu} V_{\lambda 0\lambda_1}) \chi_{\lambda_1\mu_1,\alpha\beta}^R(\omega) + V_{0000} (\delta_{\lambda 0} - \delta_{\mu 0}) \chi_{\lambda\mu,\alpha\beta}^R(\omega). \end{aligned} \quad (54)$$

Using Eq. (54) in Eq. (53) to eliminate Γ , one ultimately may write what amounts to a matrix equation for $\chi_{\lambda\mu,\alpha\beta}^R(\omega)$,

$$\begin{aligned} (\omega + \varepsilon_\mu - \varepsilon_\lambda) \chi_{\lambda\mu,\alpha\beta}^R(\omega) &= (n_\mu - n_\lambda) \delta_{\alpha\lambda} \delta_{\beta\mu} + (n_\mu - n_\lambda) \sum_{\lambda_1\mu_1} [V_{\lambda\mu_1\lambda_1\mu} + V_{\lambda\mu_1\mu\lambda_1}] \chi_{\lambda_1\mu_1,\alpha\beta}^R(\omega) \\ & \quad - (n_\mu - n_\lambda) \sum_{\lambda_1\mu_1} [V_{\lambda\mu_1\lambda_1\mu} (\delta_{\lambda_1 0} \delta_{\lambda_1\lambda} + \delta_{\mu_1 0} \delta_{\mu_1\mu}) + V_{\lambda\mu_1\mu\lambda_1} (\delta_{\lambda_1 0} + \delta_{\mu_1 0}) (\delta_{\lambda_1\lambda} + \delta_{\mu_1\mu})] \chi_{\lambda_1\mu_1,\alpha\beta}^R(\omega). \end{aligned} \quad (55)$$

Interestingly, the first line of this equation has the same form as what is obtained from the TDHFA using the standard grand-canonical ensemble, although the energies and occupations are different because of the nonlocal terms in the self-energy that arise from using the constrained grand-canonical ensemble. The terms in the second line also come from these nonlocal terms. This equation for the density response function provides a natural way to describe the coupling between the condensate and normal components through the matrix indices, which may refer to the condensate state or to the depletion states. We will illustrate this explicitly when we solve Eq. (55) for a homogenous system below.

Finally, it is useful to note that Eq. (55) can be written in the form of a Bethe-Salpeter equation

$$\chi_{\lambda\mu,\alpha\beta}^0(\omega) = \chi_{\lambda\mu,\alpha\beta}^0(\omega) + \sum_{\eta\nu\rho\sigma} \chi_{\lambda\mu,\rho\nu}^0(\omega) K_{\rho\nu,\eta\sigma}(\omega) \chi_{\eta\sigma,\alpha\beta}(\omega), \quad (56)$$

where $\chi_{\lambda\mu,\alpha\beta}^0(\omega)$ is defined

$$\chi_{\lambda\mu,\alpha\beta}^0(\omega) = \frac{n_\mu - n_\lambda}{\omega + i\eta + \varepsilon_\mu - \varepsilon_\lambda} \delta_{\alpha\lambda} \delta_{\beta\mu}, \quad (57)$$

and the kernel K ,

$$\begin{aligned} K_{\rho\nu,\eta\sigma}(\omega) &= V_{\rho\sigma\eta\nu} (1 - \delta_{\eta 0} \delta_{\rho\eta} - \delta_{\sigma 0} \delta_{\sigma\nu}) + V_{\rho\sigma\nu\eta} \\ & \quad \times [1 - (\delta_{\rho 0} + \delta_{\nu 0}) (\delta_{\eta\rho} + \delta_{\sigma\nu})] \end{aligned} \quad (58)$$

which is independent of the frequency.

Equation (55) is valid for a dilute Bose gas with any shape of static external potential $U(\vec{r})$ and a general two-body interaction potential $V(\vec{r}_1 - \vec{r}_2)$. In general it must be solved numerically. In the next section, we will show that it can be solved analytically for a uniform, homogeneous system of bosons interacting via a contact two-body interaction.

IV. APPLICATION TO A HOMOGENOUS SYSTEM

In this section, we apply the above results to discuss the single-particle and collective excitations of a homogeneous system with a contact two-body interaction, $V(\vec{r}_1 - \vec{r}_2) = g\delta(\vec{r}_1 - \vec{r}_2)$. This is a common and quantitatively accurate approximation for dilute Bose gases in many situations. We begin by reviewing the solutions of the static Hartree-Fock equations for this case [4].

A. Static Hartree-Fock for a Bose-Einstein condensate

For a uniform homogeneous system [$U(\vec{r})=0$], the Hartree-Fock Hamiltonian is diagonalized by plane waves, $\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{r}}$, with Ω the volume of the system, and the single-particle energies are easily shown to be

$$\varepsilon_{\vec{k}} = \varepsilon_{\vec{k}}^0 + 2g\rho - g\rho_0\delta_{\vec{k},0} \quad (59)$$

where $\varepsilon_{\vec{k}}^0 = \frac{\hbar^2 k^2}{2m}$, $\rho = N/\Omega$, and $\rho_0 = N_0/\Omega$. Below the critical temperature, the chemical potential is given by the lowest eigenvalue

$$\mu = \varepsilon_0 = g(2\rho - \rho_0). \quad (60)$$

Note that there is a gap in the single-particle spectrum $\Delta = g\rho_0$ with respect to the chemical potential for a Bose-condensed system. As discussed in the Introduction, if the grand-canonical ensemble is used, there is no such gap and the corresponding single-particle energy is $\varepsilon_{\vec{k}} = \varepsilon_{\vec{k}}^0 + 2g\rho$. However, the absence of the gap is an artifact of strong number fluctuations in the condensed state, which are more properly controlled by the constrained grand-canonical ensemble.

The gapped structure of the single-particle spectrum may be probed in principle via a tunneling experiment. One interesting possible approach involves a ‘‘single-atom pipette’’ that has recently been proposed [17], in which bosons are loaded into a strongly localized potential. Because of the potential well, there can be a considerable gap for excitations within the pipette, and at low temperatures all the atoms will be at the same energy. By bringing the pipette sufficiently close to the bulk BEC for a fixed time, atoms may tunnel out of the pipette into the bulk BEC, and a measurement of the number of atoms remaining in the pipette after this process allows one to infer the tunneling rate. For a relatively deep pipette potential, one expects the atoms to tunnel only into the condensate state of the BEC. As the energy is raised, however, there should be a sharp threshold energy, set by the gap, above which atoms may also tunnel into the excited states. This will show up as a nonanalytic contribution to the tunneling rate reflecting the density of depletion states in the BEC. For a bulk, three-dimensional BEC, this would be proportional to $(E - E_{th})^{1/2}$, with E the energy of the bosons in

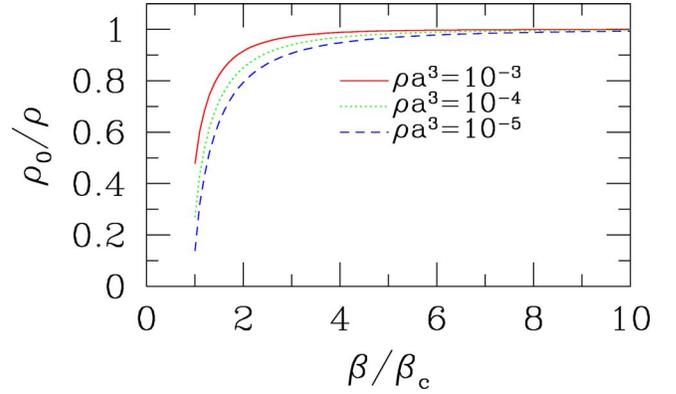


FIG. 1. (Color online) Condensation fraction as a function of the temperature at three dilute parameters.

the pipette, and E_{th} set by the gap energy. We note that the exponent might be renormalized by shakeup effects [18], but we expect the nonanalytic behavior to be robust and to reflect the gap in the single-particle spectrum.

The critical temperature T_c is determined by taking the limit $\rho_0 \rightarrow 0$, so that the number of particles depleted from the condensate tends to the total number of particles N . This leads to the condition

$$N = \frac{V}{(2\pi)^3} \int d^3\vec{k} \frac{1}{e^{\beta_c \varepsilon_{\vec{k}}^0} - 1}, \quad (61)$$

which gives [4]

$$k_B T_c = \frac{4\pi}{2m} \rho^{2/3} \left(\frac{1}{g_{3/2}(1)} \right)^{2/3}, \quad (62)$$

where

$$g_\gamma(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^\gamma}. \quad (63)$$

The condensate density ρ_0 below T_c is found by requiring depletion of the condensate to be equal to the thermal occupation of the excited states [4],

$$1 - \frac{\rho_0}{\rho} = \frac{1}{(2\pi)^3 \rho} \int d\vec{k} \frac{1}{e^{\beta(\varepsilon_{\vec{k}}^0 + g\rho_0)} - 1} = \frac{1}{\lambda_T^3 g_{3/2}(z)}, \quad (64)$$

where $z = e^{-\beta g\rho_0}$, and

$$\lambda_T' = \left(\frac{2\pi\hbar^2\beta}{m} \right)^{1/2} \rho^{1/3} = \lambda_T \rho^{1/3} \quad (65)$$

is the product of the thermal wavelength and the inverse average distance between particles. We note that although the Hartree-Fock approximation yields precisely the same T_c as for a noninteracting system, the phase transition into the condensed state is first order rather than continuous. This can be seen in the behavior of the condensation fraction as a function of the temperature, as illustrated in Fig. 1.

From Eq. (64) and Fig. 1, we can see that in the HFA, the repulsive interaction enhances the condensation relative to the noninteracting case [16].

B. Collective modes from the depletion Green's function

We would like to solve Eq. (44) for the case at hand; in order to do this we need to specify $\delta\Sigma$. For contact interactions in the homogeneous system, this is easily evaluated, with the result

$$\delta\Sigma(\vec{r}_1, \tau_1; \vec{r}_2, \tau_2) = \left\{ 2g[\delta\tilde{\rho}(\vec{r}_1, \tau_1) + \delta\rho_0(\vec{r}_1, \tau_1)]\delta(\vec{r}_1 - \vec{r}_2) + g \left[\delta w(\vec{r}_1, \vec{r}_2; \tau_1)\rho_0(\vec{r}_1, \vec{r}_2) - \frac{1}{\Omega}\delta\rho_0(\vec{r}_1, \vec{r}_2; \tau_1) \right] \right\} \delta(\tau_1 - \tau_2). \quad (66)$$

In this equation, $\delta\tilde{\rho}(\vec{r}_1, \tau_1) = \delta\tilde{G}(\vec{r}_1, \tau_1, \vec{r}_1, \tau_1^+)$ is the variation of the depleted particle density, $\delta\tilde{\rho}_0(\vec{r}_1, \tau_1) = N_0\delta W_0(\vec{r}_1, \vec{r}_1, \tau_1)$ is the variation of the condensate density, and $\delta w(\vec{r}_1, \vec{r}_2; \tau_1) = -[\delta\psi_0(\vec{r}_1) + \delta\psi_0^*(\vec{r}_1) + \psi_0(\vec{r}_2) + \delta\psi_0^*(\vec{r}_2)]/\sqrt{\Omega}$. As in the case of the density response function, we can make progress by expanding the various quantities in terms of the unperturbed single particle states. Thus we define $\delta\tilde{G}_{\vec{k}_1, \vec{k}_2}(i\omega_1, i\omega_2)$ via

$$\delta\tilde{G}(\vec{r}_1, \tau_1, \vec{r}_2, \tau_2) = \frac{1}{\beta^2} \sum_{i\omega_1, i\omega_2} e^{-i\omega_1\tau_1 + i\omega_2\tau_2} \frac{1}{\Omega} \sum_{\vec{k}_1, \vec{k}_2} e^{i\vec{k}_1\cdot\vec{r}_1 - i\vec{k}_2\cdot\vec{r}_2} \delta\tilde{G}_{\vec{k}_1, \vec{k}_2}(i\omega_1, i\omega_2). \quad (67)$$

It is useful to notice that the Fourier transform of the depletion density, $\delta\tilde{\rho}(\vec{k}, i\omega_n) = \int_0^\beta d\tau \int d\vec{r} e^{i\vec{k}\cdot\vec{r} + i\omega_n\tau} \delta\tilde{\rho}(\vec{r}, \tau)$, satisfies

$$\delta\tilde{\rho}(\vec{k}, i\omega_n) = \frac{1}{\Omega\beta} \sum_{i\omega'_n, \vec{k}'} \delta\tilde{G}_{\vec{k}+\vec{k}', \vec{k}'}(i\omega_n + i\omega'_n, i\omega'_n). \quad (68)$$

Using Eq. (67), Eq. (44) may be recast in a particularly simple form. For $\vec{k}_1, \vec{k}_2 \neq 0$, we find

$$[\varepsilon_{\vec{k}_1} - i\omega_1][\varepsilon_{\vec{k}_2} - i\omega_2] \delta\tilde{G}_{\vec{k}_1, \vec{k}_2}(i\omega_1, i\omega_2) + \frac{2g}{\Omega\beta} \sum_{\vec{k}', i\omega'} \delta\tilde{G}_{\vec{k}'+\Delta\vec{k}, \vec{k}'}(i\omega' + i\Delta\omega, i\omega') + 2g\delta\rho_0(\Delta\vec{k}, i\Delta\omega) = -\delta U(\Delta\vec{k}, i\Delta\omega), \quad (69)$$

where $\Delta\omega = \omega_1 - \omega_2$, $\Delta\vec{k} = \vec{k}_1 - \vec{k}_2$, and

$$\delta\rho_0(\Delta\vec{k}, i\Delta\omega_n) = \frac{1}{\Omega} \int_0^\beta d\tau \int d\vec{r} e^{i\Delta\vec{k}\cdot\vec{r} + i\Delta\omega_n\tau} \times [\delta\psi_0(\vec{r}, \tau) + \delta\psi_0^*(\vec{r}, \tau)]$$

$$\delta U(\Delta\vec{k}, i\Delta\omega_n) = \frac{1}{\Omega} \int_0^\beta d\tau \int d\vec{r} e^{i\Delta\vec{k}\cdot\vec{r} + i\Delta\omega_n\tau} \delta U(\vec{r}, \tau).$$

It is clear that in Eq. (69) we would like to write $\vec{k}_1 = \vec{k}_2 + \Delta\vec{k}$, $\omega_1 = \Delta\omega + \omega_2$, divide by the equation by $[\varepsilon_{\vec{k}_1} - i\omega_1][\varepsilon_{\vec{k}_2} - i\omega_2]$ and sum with respect to \vec{k}_1 and ω_1 . However, there is a caveat: in doing this our indices run over $k_1=0$ and $k_2=0$, which introduces further terms in Eq. (69). It is not difficult

to show that these terms vanish in the thermodynamic limit ($\Omega \rightarrow \infty$), which is the case of interest to us. Performing the above steps, Eq. (69) becomes a simple linear equation,

$$\left[\frac{1}{\tilde{P}(\Delta\vec{k}, i\Delta\omega)} - 2g \right] \delta\tilde{\rho}(\Delta\vec{k}, i\Delta\omega) - 2g\delta\rho_0(\Delta\vec{k}, i\Delta\omega) = \delta U(\Delta\vec{k}, i\Delta\omega), \quad (70)$$

where $\tilde{P}(\vec{q}, i\omega_n) = \frac{1}{\Omega} \sum_{\vec{k}}' [n_B(\tilde{\varepsilon}_{\vec{k}+\vec{q}}) - n_B(\tilde{\varepsilon}_{\vec{k}})] / [i\omega_n + \tilde{\varepsilon}_{\vec{k}+\vec{q}} - \tilde{\varepsilon}_{\vec{k}}]$, $\tilde{\varepsilon}_{\vec{k}} = \varepsilon_{\vec{k}} - \mu$, $n_B(\varepsilon) = 1/(e^{\beta\varepsilon} - 1)$ is the Bose occupation factor, and the prime on the sum indicates that $\vec{k}, \vec{k}+\vec{q}=0$ should not be included.

Since the problem involves two density disturbances, the depletion density $\delta\tilde{\rho}$ and the condensate density $\delta\rho_0$, we need a second equation. This can be obtained directly from the ground-state wave function disturbance, as described in Appendix B, since $\delta\rho_0(\vec{r}, \tau) = \frac{N_0}{\sqrt{\Omega}} [\delta\psi_0(\vec{r}, \tau) + \delta\psi_0^*(\vec{r}, \tau)]$. Using the method of Appendix B, one may easily show for imaginary time,

$$\delta\psi_0(\vec{r}, i\omega_n) = \frac{1}{\Omega^{3/2}} \sum_{\vec{k}}' \left[\frac{\delta U(\vec{k}, i\omega_n) + \delta\Sigma(\vec{k}, i\omega_n)}{i\omega_n - \tilde{\varepsilon}_{\vec{k}}} \right] e^{i\vec{k}\cdot\vec{r}}, \quad (71)$$

where the prime on the sum indicates $\vec{k}=0$ should not be included, and

$$\delta\Sigma(\vec{k}, i\omega_n) = \int d\vec{r}_1 d\vec{r}_2 \int d\tau_1 d\tau_2 e^{i\omega_n\tau_1 + i\vec{k}\cdot\vec{r}_1} \delta\Sigma(\vec{r}_1, \tau_1, \vec{r}_2, \tau_2). \quad (72)$$

Substituting Eq. (66) into Eq. (71), one obtains

$$\delta\psi_0(\vec{k}, i\omega_n) = \frac{1}{i\omega_n - \tilde{\varepsilon}_{\vec{k}}} \left[\frac{1}{\sqrt{\Omega}} \delta U(\vec{k}, i\omega_n) + \frac{2g}{\sqrt{\Omega}} \delta\tilde{\rho}(\vec{k}, i\omega_n) + g\rho_0 \delta\psi_0^*(\vec{k}, i\omega_n) \right], \quad (73)$$

where $\delta\psi_0(\vec{k}, i\omega_n) = \int d\vec{r} \int d\tau e^{i\vec{k}\cdot\vec{r}} \delta\psi_0(\vec{r}, \tau)$ and $\delta\psi_0^*(\vec{k}, i\omega_n) = \int d\vec{r} \int d\tau e^{i\vec{k}\cdot\vec{r}} \delta\psi_0^*(\vec{r}, \tau)$. Similarly, one finds

$$\delta\psi_0^*(\vec{k}, i\omega_n) = \frac{1}{-i\omega_n - \tilde{\varepsilon}_{\vec{k}}} \left[\frac{1}{\sqrt{\Omega}} \delta U(\vec{k}, i\omega_n) + \frac{2g}{\sqrt{\Omega}} \delta\tilde{\rho}(\vec{k}, i\omega_n) + g\rho_0 \delta\psi_0(\vec{k}, i\omega_n) \right]. \quad (74)$$

Equations (73) and (74) may be substituted into the definition of $\delta\rho_0$ to obtain

$$\left[\frac{(i\omega_n)^2}{\tilde{\varepsilon}_{\vec{k}} - g\rho_0} - \tilde{\varepsilon}_{\vec{k}} - g\rho_0 \right] \delta\rho_0(\vec{k}, i\omega_n) - 4g\rho_0 \delta\tilde{\rho}(\vec{k}, i\omega_n) = 2g\rho_0 \delta U(\vec{k}, i\omega_n), \quad (75)$$

providing the second equation needed to compute the density disturbance.

Equations (70) and (75) may be combined into a single matrix equation,

$$\begin{pmatrix} \frac{1}{\tilde{P}(\vec{q}, i\omega_n)} - 2g & -2g \\ -2g & \frac{1}{2\rho_0} \left[\frac{(i\omega_n)^2}{\tilde{\varepsilon}_{\vec{q}} - g\rho_0} - (\tilde{\varepsilon}_{\vec{q}} + g\rho_0) \right] \end{pmatrix} \times \begin{pmatrix} \delta\tilde{\rho}(\vec{q}, i\omega_n) \\ \delta\rho_0(\vec{q}, i\omega_n) \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \delta U(\vec{q}, i\omega_n). \quad (76)$$

Collective modes of the system propagate when $\delta\tilde{\rho}$, $\delta\rho_0 \neq 0$ even if $\delta U=0$. This is only possible if the matrix on the left hand side of Eq. (76) has vanishing determinant,

$$\left[\frac{1}{\tilde{P}(\vec{q}, i\omega_n)} - 2g \right] \left[\frac{(i\omega_n)^2}{\tilde{\varepsilon}_{\vec{q}} - g\rho_0} - (\tilde{\varepsilon}_{\vec{q}} + g\rho_0) \right] - 8g^2\rho_0 = 0. \quad (77)$$

Upon analytic continuation ($i\omega_n \rightarrow \omega + i\eta$), Eq. (77) supports a linearly dispersing gapless mode (zero sound) for any $\rho_0 \neq 0$, as expected for an infinite uniform superfluid. This is a nontrivial check that our formalism obtains physically sensible results. Before analyzing this in further detail, we demonstrate that the same result may be obtained directly from the linear response formalism. While somewhat more complex to carry through, this latter approach allows us to look at very general response functions, and so yields more information than the density responses above.

C. Density-density response function and collective excitations

Our starting point for this analysis is Eq. (55). For a homogenous system, χ^R vanishes unless the indices are such that momentum conservation is respected. Thus we may set $\lambda = \vec{k}_1 - \vec{q}/2$, $\mu = \vec{k}_1 + \vec{q}/2$, $\alpha = \vec{k}_2 - \vec{q}/2$, and $\beta = \vec{k}_2 + \vec{q}/2$. Denoting

$$\chi_{\vec{k}_1\vec{k}_2}^R(\vec{q}; \omega) = \chi_{\vec{k}_1 - (\vec{q}/2)\vec{k}_1 + \vec{q}/2, \vec{k}_2 - (\vec{q}/2)\vec{k}_2 + \vec{q}/2}^R(\omega), \quad (78)$$

one obtains

$$\begin{aligned} & [\omega + \varepsilon_{\vec{k}_1 + \vec{q}/2} - \varepsilon_{\vec{k}_1 - \vec{q}/2}] \chi_{\vec{k}_1\vec{k}_2}^R(\vec{q}; \omega) \\ &= (n_{\vec{k}_1 + \vec{q}/2} - n_{\vec{k}_1 - \vec{q}/2}) \delta_{\vec{k}_1\vec{k}_2} + (n_{\vec{k}_1 + \vec{q}/2} - n_{\vec{k}_1 - 1/2\vec{q}}) \\ &\quad \times \frac{2g}{\Omega} \sum_{\vec{k}_3} \chi_{\vec{k}_3\vec{k}_2}^R(\vec{q}; \omega) - g\rho_0 (\delta_{\vec{k}_1 - (\vec{q}/2)} - \delta_{\vec{k}_1, (\vec{q}/2)}) \\ &\quad \times [\chi_{(\vec{q}/2)\vec{k}_2}^R(\vec{q}; \omega) + \chi_{-(\vec{q}/2)\vec{k}_2}^R(\vec{q}; \omega)] \\ &\quad - g\rho_0 (\delta_{\vec{k}_1, -\vec{q}/2} - \delta_{\vec{k}_1, \vec{q}/2}) \chi_{\vec{k}_1\vec{k}_2}^R(\vec{q}; \omega). \end{aligned} \quad (79)$$

Bringing the last term to the left side of the equation has the interesting effect of canceling the gap in the single-particle spectrum, since

$$\varepsilon_{\vec{k}_1 + \vec{q}/2} - \varepsilon_{\vec{k}_1 - \vec{q}/2} + g\rho_0 (\delta_{\vec{k}_1, -\vec{q}/2} - \delta_{\vec{k}_1, \vec{q}/2}) = \varepsilon_{\vec{k}_1 + (\vec{q}/2)}^0 - \varepsilon_{\vec{k}_1 - (\vec{q}/2)}^0, \quad (80)$$

where $\varepsilon_{\vec{k}}^0 = \frac{\hbar^2 \vec{k}^2}{2m}$ is the free single-particle energy. This cancellation is only possible because our linear response equation was generated in a way that is consistent with the self-energy used in the static Hartree-Fock analysis [10].

Using Eq. (79), one can obtain

$$\begin{aligned} & [\chi_{(\vec{q}/2)\vec{k}_2}^R(\vec{q}; \omega) + \chi_{-(\vec{q}/2)\vec{k}_2}^R(\vec{q}; \omega)] \\ &= \frac{\omega^2 - (\varepsilon_{\vec{q}}^0)^2}{\omega^2 - (\varepsilon_{\vec{q}}^0)^2 + 2g\rho_0\varepsilon_{\vec{q}}^0} \left[\frac{N_0 - n_{\vec{q}}}{\omega - \varepsilon_{\vec{q}}^0} \delta_{\vec{k}_2, -\vec{q}/2} - \frac{N_0 - n_{\vec{q}}}{\omega + \varepsilon_{\vec{q}}^0} \delta_{\vec{k}_2, \vec{q}/2} \right] \\ &\quad + \frac{2(N_0 - n_{\vec{q}})\varepsilon_{\vec{q}}^0}{\omega^2 - (\varepsilon_{\vec{q}}^0)^2 + 2g\rho_0\varepsilon_{\vec{q}}^0} \frac{2g}{\Omega} \sum_{\vec{k}_3} \chi_{\vec{k}_3\vec{k}_2}^R(\vec{q}; \omega). \end{aligned} \quad (81)$$

Substituting this result back into Eq. (79) leads to

$$\begin{aligned} \chi_{\vec{k}_1\vec{k}_2}^R(\vec{q}; \omega) &= \frac{n_{\vec{k}_1 + \vec{q}/2} - n_{\vec{k}_1 - \vec{q}/2}}{\omega + \varepsilon_{\vec{k}_1 + \vec{q}/2}^0 - \varepsilon_{\vec{k}_1 - \vec{q}/2}^0} \delta_{\vec{k}_1\vec{k}_2} - \frac{g}{\Omega} \frac{N_0 \delta_{\vec{k}_1, -\vec{q}/2} - N_0 \delta_{\vec{k}_1, \vec{q}/2}}{\omega + \varepsilon_{\vec{k}_1 + \vec{q}/2}^0 - \varepsilon_{\vec{k}_1 - \vec{q}/2}^0} \frac{\omega^2 - (\varepsilon_{\vec{q}}^0)^2}{\omega^2 - (\varepsilon_{\vec{q}}^0)^2 + 2g\rho_0\varepsilon_{\vec{q}}^0} \left[\frac{N_0 - n_{\vec{q}}}{\omega - \varepsilon_{\vec{q}}^0} \delta_{\vec{k}_2, -\vec{q}/2} - \frac{N_0 - n_{\vec{q}}}{\omega + \varepsilon_{\vec{q}}^0} \delta_{\vec{k}_2, \vec{q}/2} \right] \\ &\quad + \left[\frac{n_{\vec{k}_1 + \vec{q}/2} - n_{\vec{k}_1 - \vec{q}/2}}{\omega + \varepsilon_{\vec{k}_1 + \vec{q}/2}^0 - \varepsilon_{\vec{k}_1 - \vec{q}/2}^0} - \frac{g}{\Omega} \frac{N_0 \delta_{\vec{k}_1, -\vec{q}/2} - N_0 \delta_{\vec{k}_1, \vec{q}/2}}{\omega + \varepsilon_{\vec{k}_1 + \vec{q}/2}^0 - \varepsilon_{\vec{k}_1 - \vec{q}/2}^0} \frac{2(N_0 - n_{\vec{q}})\varepsilon_{\vec{q}}^0}{\omega^2 - (\varepsilon_{\vec{q}}^0)^2 + 2g\rho_0\varepsilon_{\vec{q}}^0} \right] \frac{2g}{\Omega} \sum_{\vec{k}_3} \chi_{\vec{k}_3\vec{k}_2}^R(\vec{q}; \omega). \end{aligned} \quad (82)$$

Now summing over \vec{k}_1 and \vec{k}_2 , one gets

$$\begin{aligned} \chi_{nm}^R(\vec{q}; \omega) &= \tilde{P}(\vec{q}; \omega) + \frac{2\rho_0\varepsilon_{\vec{q}}^0}{\omega^2 - (\varepsilon_{\vec{q}}^0)^2 + 2g\rho_0\varepsilon_{\vec{q}}^0} + 2g \left[\tilde{P}(\vec{q}; \omega) \right. \\ &\quad \left. + \frac{2\rho_0\varepsilon_{\vec{q}}^0}{\omega^2 - (\varepsilon_{\vec{q}}^0)^2 + 2g\rho_0\varepsilon_{\vec{q}}^0} \right] \chi_{nm}^R(\vec{q}; \omega). \end{aligned} \quad (83)$$

One finally may express $\chi_{nm}^R(\vec{q}; \omega)$ in a symmetric form,

$$\chi_{nm}^R(\vec{q}; \omega) = \frac{\tilde{P}(\vec{q}; \omega) + P_c(\vec{q}; \omega)}{1 - 2g[\tilde{P}(\vec{q}; \omega) + P_c(\vec{q}; \omega)]}, \quad (84)$$

where we have denoted

$$P_c(\vec{q}; i\omega) = \frac{2\rho_0 \varepsilon_q^0}{\omega^2 - (\varepsilon_q^0)^2 + 2g\rho_0 \varepsilon_q^0}, \quad (85)$$

which can be interpreted as the polarization function for the condensate. The poles of χ_{mn} determine the collective modes, and are given by solutions to

$$1 = 2g[\tilde{P}(\vec{q}; \omega) + P_c(\vec{q}; i\omega)]. \quad (86)$$

It is not difficult to show that this is identical to Eq. (77).

D. Discussion

Several comments about the linear response results as obtained from our TDHFA approach are in order. Firstly, at $T=0$, $\tilde{P}(\vec{q}; \omega)=0$, and the density-density response function becomes

$$\chi_{mn}(\vec{q}; \omega, T=0) = \frac{P_c(\vec{q}; \omega)}{1 - 2gP_c(\vec{q}; \omega)}, \quad (87)$$

with the pole given by

$$\omega^2(\vec{q}, T=0) = 2g\rho\varepsilon_q^0 + (\varepsilon_q^0)^2. \quad (88)$$

This is exactly the same as that obtained by linearizing the time-dependent GP equation.

This result, as in the Bogoliubov spectrum, evolves from a soundlike (linear in q) form to a particlelike ($\sim q^2$) with increasing q . Nevertheless, this mode does not involve a change in particle number for any value of q . The particlelike spectrum arises at large q because of the admixture of a finite momentum component into the condensate wave function, whose energy is dominated by the kinetic rather than interaction energy at large q . In addition to the collective mode spectrum, we expect a separate branch of single-particle excitations which involve changing the total particle number of the system, and also has a q^2 dispersion at high momentum.

Secondly, we note that Eq. (86) yields a propagating gapless mode for *any* $\rho_0 \neq 0$. This means our approach correctly captures the superfluid mode of the system whenever it is Bose-condensed. Thus in retaining the correct (gapped) structure for the single-particle excitations, we see that the gapless superfluid mode is not sacrificed. At $T > T_c$, $P_c(\vec{q}; \omega)=0$, and writing $\tilde{P}=P$, the density-density response function is

$$\chi_{mn}(\vec{q}; \omega) = \frac{P(\vec{q}; \omega)}{1 - 2gP(\vec{q}; \omega)}, \quad (89)$$

with poles determined by

$$1 = 2gP(\vec{q}; \omega), \quad (90)$$

which is the known result for the normal Bose gas [19].

Thirdly, because of the structure of Eqs. (76) and (86), one might expect to find two collective modes, one in which the condensate and depleted particle densities oscillate in phase, and the other in which they are out of phase. These would correspond to zero and second sound, respectively. We find, however, that for attainable values of $\mu(T)$ and

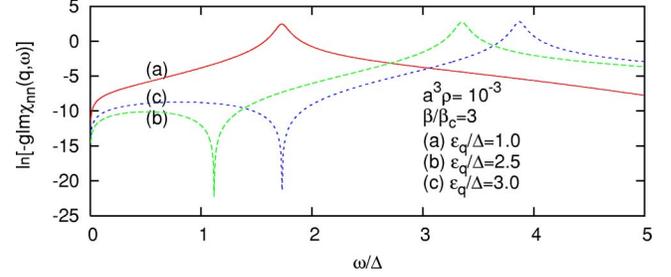


FIG. 2. (Color online) Imaginary part of the density response for different values of q as a function of ω for a Bose condensate at inverse temperature β (in units of the inverse critical temperature β_c) with density ρ and scattering length $a \equiv m/4\pi\hbar^2g$.

$\rho_0(T)$ within the HFA, the two solutions of Eq. (86) occur with one at positive ω^2 and the other at a negative value; the second sound mode is thus overdamped. This is similar to the weak coupling limit [7]. However, unlike the weak coupling limit, here the second sound is overdamped because of the gap in the single-particle spectrum, which makes the depletion particle density too small to support a propagating second sound mode. The gap has another interesting effect on the interaction between the condensate and depleted particles. This is illustrated in Fig. 2, which depicts the imaginary part of the density response function, $\chi_{mn}(q, \omega + i\eta)$ for fixed q as a function of ω . Two features are prominently visible: a peak (which becomes a delta function in the limit $q \rightarrow 0$) representing the superfluid mode, and a zero in the response that appears for $q^2/2m > 2\Delta \equiv 2g\rho_0$. The width of the superfluid mode arises because of the interaction of the condensate with the depletion particles, and vanishes at low temperature as $e^{-\Delta/k_B T}$. Note we can obtain this temperature dependence *only* because our choice of self-energy creates a gap between the condensate and excited states, even though we use a single Hamiltonian to describe them. The zero arises when $\omega^2 = (\frac{q^2}{2m})(\frac{q^2}{2m} - 2\Delta)$, and represents a frequency at which $\delta\tilde{\rho}$ in Eq. (76) vanishes. In this situation the condensate precisely screens the perturbing potential δU for the depletion particles. Since the depleted particles are unperturbed and the condensate cannot absorb energy away from the superfluid frequency, no energy can be absorbed by the system, leading to the zero. It is interesting to note that an observation of this effect would allow one to measure the energy gap of the system.

Finally, for small depletions $\tilde{\rho}$, the velocity of the zero sound mode found from Eq. (86) may be shifted either upward or downward, depending on the numerical value of the gas parameter. This is most easily demonstrated by expanding the equation for small $\tilde{\rho}$ and small \tilde{P} . The correction to the sound velocity can then be shown to have the form $\delta c_0 = \frac{1}{4mc_0}\{g\Delta\rho_0 + 8g^2\rho\tilde{P}_0\}$, where c_0 is the zero sound velocity at zero temperature, $\Delta\rho_0$ the change in the condensate from its zero temperature value, and $\tilde{P}_0 = \lim_{q \rightarrow 0} \tilde{P}_q(\omega = c_0 q)$. For small values of ρ , $\tilde{P}_0 < 0$, and the mode velocity decreases with temperature, as is commonly found in the Bogoliubov approximation. By contrast, we find for larger values $\tilde{P}_0 > 0$, and for large enough ρ , its value is sufficiently large to

render $\delta c_0 > 0$. This means relatively dense superfluids may have increasing zero sound velocity with temperature, as is found in the random phase approximation and appears to be consistent with data for ^4He [20]. That the TDHFA can capture both these limiting behaviors demonstrates the utility of the method.

V. CONCLUSION

In this work, we demonstrated that the TDHFA may be developed in a way that does not break the gauge symmetry of the Hamiltonian, thus allowing us to correctly obtain a gapped single-particle spectrum, and yet correctly produces a gapless superfluid mode in the collective response of an infinite uniform system. By developing both the depletion Green's function and response functions, we can examine the single-particle and collective mode spectra separately. The key to obtaining these features in a consistent way was to retain the nonlocal terms in the self-energy [see Eqs. (33) and (41)], which were required by the orthogonality of the single-particle wave functions, and ultimately lead to a precise cancellation of the gap in the single-particle energies when we calculate the density response function [Eq. (80)].

Finally, we point out that our equations for the infinite uniform system [Eq. (76)] are formally similar to equations for the density response obtained using ensembles in which the gauge symmetry is broken [6]. This formal similarity however does not generally occur; for example if we had studied a uniform but finite size system (particles in a box), we would find further terms that vanish in the thermodynamic limit, which do not appear in other approaches. Generally speaking, in computing collective modes of a Bose condensate, the challenge is to find how the condensate density couples to the depleted particles in a way that is conserving [10], and preserves the gapless mode expected for an infinite system [5]. As discussed above, the TDHFA is guaranteed to be conserving as it is controlled by a single Hamiltonian (in contrast to many other methods), and we have demonstrated that it correctly produces the expected superfluid mode. Beyond the case we studied in detail in presenting our method here, the TDHFA can be used to study inhomogeneous and/or finite size systems, and may be very naturally generalized to handle multicomponent Bose systems, rotating systems, and even boson-fermion mixtures. Future studies will focus on these applications.

ACKNOWLEDGMENTS

This work was supported by the NSF Grant No. DMR0454699. The authors thank Allan Griffin and Wei Zhang for useful comments and discussions.

APPENDIX A: PROOF OF EQ. (28)

The off diagonal matrix elements of Σ can be found by varying the orthogonal basis ψ_α . We assume that $|\Psi\rangle$ is a Hartree-Fock permanent constructed from orthonormal single-particle states ψ_α , which can be expressed

$$|\Psi\rangle = \prod_j \frac{(a_\alpha^\dagger)^{n_{\alpha_j}}}{\sqrt{n_{\alpha_j}!}} |0\rangle, \quad (\text{A1})$$

where $|0\rangle$ is a vacuum state. The variation of the single-particle states may be written

$$\delta\psi_\alpha = \sum_\gamma \eta_{\alpha\gamma} \psi_\gamma \quad \text{or} \quad \delta a_\alpha^\dagger = \sum_\gamma \eta_{\alpha\gamma} a_\gamma^\dagger, \quad (\text{A2})$$

with the orthonormality of the basis ψ_α implying that [11]

$$\eta_{\alpha\beta} + \eta_{\beta\alpha}^* = 0. \quad (\text{A3})$$

We can prove that the change of the permanent (A1) due to the basis change (A2) can be generally expressed as follows:

$$|\delta\Psi\rangle = \sum_{\alpha\beta} \eta_{\alpha\beta} a_\beta^\dagger a_\alpha |\Psi\rangle. \quad (\text{A4})$$

This can be shown by substituting Eq. (A2) into Eq. (A1),

$$|\delta\Psi\rangle = \sum_{i,\beta} \eta_{\alpha_i\beta} \prod_{j \neq i,\beta} \frac{(a_\alpha^\dagger)^{n_{\alpha_j}}}{\sqrt{n_{\alpha_j}!}} (a_\alpha^\dagger)^{n_{\alpha_i}-1} \frac{n_{\alpha_i}}{\sqrt{n_{\alpha_i}}} a_\beta^\dagger |0\rangle. \quad (\text{A5})$$

Now moving a_β^\dagger to the left side and noticing $\frac{n_{\alpha_i}}{\sqrt{n_{\alpha_i}}} (a_\alpha^\dagger)^{n_{\alpha_i}-1} |0\rangle = \sqrt{n_{\alpha_i}} |n_{\alpha_i}-1\rangle = a_{\alpha_i} |n_{\alpha_i}\rangle$, one obtains Eq. (A4).

The change of the free energy due to the basis change is

$$\delta\Omega = \frac{\sum_i' e^{-\beta(E_i - \mu N)} [\langle \delta\Psi_i | H | \Psi_i \rangle + \langle \Psi_i | H | \delta\Psi \rangle]}{\sum_i' e^{-\beta(E_i - \mu N)}}, \quad (\text{A6})$$

where E_i is the unperturbed Hartree-Fock energy corresponding to the Ψ_i . Now substituting Eq. (A4) into the above, one obtains

$$\begin{aligned} \delta\Omega &= \sum_{\mu \neq \nu} \eta_{\nu\mu} \frac{\sum_i e^{-\beta(E_i - \mu N)} \langle \Psi_i | [H, a_\mu^\dagger a_\nu] | \Psi_i \rangle}{\sum_i e^{-\beta(E_i - \mu N)}} \\ &= \sum_{\mu \neq \nu} \eta_{\nu\mu} \langle [H, a_\mu^\dagger a_\nu] \rangle, \end{aligned} \quad (\text{A7})$$

which is the result of Eq. (28).

APPENDIX B: PERTURBATION THEORY FOR WAVE FUNCTIONS

In this appendix, we seek a formal perturbation solution of the TDHF equation since we need a relation of the functional derivative of W_α with respect to δU .

If the time-dependent external field $\delta U(\vec{r}t)$ is weak, we can solve the time-dependent single-particle wave functions $\phi_\alpha(\vec{r}t)$ using time-dependent perturbation theory. In order to do this, we expand the time-dependent single-particle wave function $\phi_\alpha(\vec{r}t)$ in terms of the static HF basis $\psi_\alpha(\vec{r})$ for times $t > t_0 \rightarrow -\infty$ as follows:

$$\phi_\alpha(\vec{r}t; \delta U) = \sum_\beta C_{\alpha\beta}(t) e^{-i\varepsilon\beta t} \psi_\beta(\vec{r}). \quad (\text{B1})$$

We seek a solution for $C_{\alpha\beta}(t)$ up to the first order of $\delta U(t)$. Substituting this into Eq. (45), after expanding the self-energy Σ to first order of $\delta U(\vec{r}t)$ and using Eq. (36), one has

$$\begin{aligned} \sum_\beta i \frac{dC_{\alpha\beta}(t_1)}{dt_1} e^{-i\varepsilon\beta t_1} \psi_\beta(\vec{r}_1) &= \delta U(\vec{r}_1 t_1) \sum_\beta C_{\alpha\beta}(t_1) e^{-i\varepsilon\beta t_1} \psi_\beta(\vec{r}_1) \\ &+ \sum_\beta C_{\alpha\beta}(t_1) e^{-i\varepsilon\beta t_1} \int d\vec{r}_2 dt_2 d\vec{r}_3 \int_{-\infty}^{t_1} dt_3 \left. \frac{\delta \Sigma(\vec{r}_1 t_1, \vec{r}_2 t_2, \delta U)}{\delta U(\vec{r}_3 t_3)} \right|_{\delta U=0} \delta U(\vec{r}_3 t_3) \psi_\beta(\vec{r}_2). \end{aligned} \quad (\text{B2})$$

We can rewrite Eq. (B2) as follows:

$$\begin{aligned} \sum_\beta i \frac{dC_{\alpha\beta}(t_1)}{dt_1} e^{-i\varepsilon\beta t_1} \psi_\beta(\vec{r}_1) &= \delta U(\vec{r}_1 t_1) \sum_\beta C_{\alpha\beta}(t_1) e^{-i\varepsilon\beta t_1} \psi_\beta(\vec{r}_1) \\ &+ \sum_\beta C_{\alpha\beta}(t_1) e^{-i\varepsilon\beta t_1} \int d\vec{r}_2 d\vec{r}_3 \int_{-\infty}^{\infty} dt_3 \Gamma^R(\vec{r}_1 \vec{r}_3, \vec{r}_2 \vec{r}_3, t_1 - t_3) \delta U(\vec{r}_3 t_3) \psi_\beta(\vec{r}_2). \end{aligned} \quad (\text{B3})$$

Multiplying both sides of Eq. (B3) by $\psi_\gamma^*(\vec{r}_1)$, integrating over \vec{r}_1 , and using the Fourier expansion

$$\delta U(\vec{r}t) = \int \frac{d\omega}{2\pi} \delta U(\vec{r}; \omega) e^{-i\omega t}, \quad (\text{B4})$$

one gets

$$\begin{aligned} i \frac{dC_{\alpha\beta}(t_1)}{dt_1} &= \sum_\gamma \int \frac{d\omega}{2\pi} C_{\alpha\gamma}(t_1) e^{-i(\omega + \varepsilon_\gamma - \varepsilon_\beta)t_1} \left[\langle \beta | \delta U(\omega) | \gamma \rangle \right. \\ &+ \left. \sum_{\lambda\mu} \Gamma_{\beta\gamma, \lambda\mu}^R(\omega) \langle \lambda | \delta U(\omega) | \mu \rangle \right]. \end{aligned} \quad (\text{B5})$$

Writing

$$C_{\alpha\beta}(t) = \delta_{\alpha\beta} + C_{\alpha\beta}^{(1)}(t) + \mathcal{O}(\delta U^2), \quad (\text{B6})$$

one finds to first order

$$\begin{aligned} i \frac{dC_{\alpha\beta}^{(1)}(t_1)}{dt_1} &= \int \frac{d\omega}{2\pi} e^{-i(\omega + \varepsilon_\alpha - \varepsilon_\beta)t_1} \left[\langle \beta | \delta U(\omega) | \alpha \rangle + \sum_{\lambda\mu} \Gamma_{\beta\alpha, \lambda\mu}^R(\omega) \right. \\ &\times \left. \langle \lambda | \delta U(\omega) | \mu \rangle \right]. \end{aligned} \quad (\text{B7})$$

Integrating this equation and using the boundary condition

$$C_{\alpha\beta}^{(1)}(t \rightarrow -\infty) = 0 \quad (\text{B8})$$

one gets

$$\begin{aligned} C_{\alpha\beta}^{(1)}(t) &= \int \frac{d\omega}{2\pi} \frac{e^{-i(\omega + \varepsilon_\alpha - \varepsilon_\beta)t}}{\omega + \varepsilon_\alpha - \varepsilon_\beta} \left[\langle \beta | \delta U(\omega) | \alpha \rangle + \sum_{\lambda\mu} \Gamma_{\beta\alpha, \lambda\mu}^R(\omega) \right. \\ &\times \left. \langle \lambda | \delta U(\omega) | \mu \rangle \right]. \end{aligned} \quad (\text{B9})$$

We finally arrive at the time-dependent Hartree-Fock single-particle wave functions up to the first order of δU ,

$$\begin{aligned} \phi_\alpha(\vec{r}t; \delta U) &= e^{-i\varepsilon_\alpha t} \left\{ \psi_\alpha(\vec{r}) + \sum_\beta \int \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\omega + \varepsilon_\alpha - \varepsilon_\beta} \left[\langle \beta | \delta U(\omega) | \alpha \rangle + \sum_{\lambda\mu} \Gamma_{\beta\alpha, \lambda\mu}^R(\omega) \langle \lambda | \delta U(\omega) | \mu \rangle \right] \psi_\beta(\vec{r}) \right\}, \\ \phi_\alpha^*(\vec{r}t; \delta U) &= e^{i\varepsilon_\alpha t} \left\{ \psi_\alpha^*(\vec{r}) + \sum_\beta \int \frac{d\omega}{2\pi} \frac{e^{i\omega t}}{\omega + \varepsilon_\alpha - \varepsilon_\beta} \left[\langle \beta | \delta U(\omega) | \alpha \rangle^* + \sum_{\lambda\mu} \Gamma_{\beta\alpha, \lambda\mu}^{R*}(\omega) \langle \lambda | \delta U(\omega) | \mu \rangle^* \right] \psi_\beta^*(\vec{r}) \right\}. \end{aligned} \quad (\text{B10})$$

The second terms of these equations are respectively the variations $\delta\psi_\alpha(\vec{r}, t)$ and $\delta\psi_\alpha^*(\vec{r}, t)$.

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