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Hartree-Fock theory for Bose-Einstein condensates and the inclusion of correlation effects

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I specialize the Hartree-Fock, random-phase, and configuration-interaction approximations to a system of interacting bosons in an external potential. This approach affords a more direct connection to the methods and language of atomic-structure calculations. The derivations and equations parallel those found in atomic structure and are contrasted with the more commonly used Bogoliubov approach for bosons. I present a numerical method for solving the Hartree-Fock and random-phase equations to obtain the low-lying excitation energies for trapped alkali-metal atoms. [S1050-2947(97)02802-3]

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I. INTRODUCTION

The recent experimental observations of Bose-Einstein condensates [1–3] and the successful experiments [4,5] on condensate properties have increased the desirability of formulating a comprehensive theoretical description. Several groups [6–14] have made progress in this direction by adopting the standard Bogoliubov approach for many interacting bosons [15]. This is an approach which treats the condensate as a reservoir which can exchange both particles and energy with the rest of the system. This approximation, however, does not inherently conserve the number of particles, although the chemical potential μ can be introduced to enforce this condition on average.

In order to connect to many-body approaches such as those used in atomic-structure calculations, I formulate the theory for trapped atoms using standard Schrödinger quantum mechanics [16]. This, of course, automatically conserves the number of interacting particles. In my methodology I pursue the analogy of atoms in a trap to electrons trapped by the Coulomb field of a nucleus. A fundamental difference between these cases is, of course, the character of the particles: the atoms experimentally studied in such traps to date are bosons, whose exchange properties differ profoundly from the fermionic electrons in an atom. This viewpoint allows me to discuss concepts such as quasiparticles in terms of *configurations* and *orbitals*, thus permitting me to link the language of condensed matter physics to that of atomic physics and nuclear physics. As I will show below, this formulation leads to results which are *largely* equivalent to those obtained in the Bogoliubov approach, aside from very minor differences that should be unimportant for current experimental conditions. A key byproduct of my viewpoint is that it permits me to apply standard tools of atomic theory, such as configuration interaction [17], which transcend Hartree-Fock theory, in order to describe phenomena such as multiple-particle excitations which are not encompassed by Bogoliubov theory.

In Sec. II, I review the essentials of second quantization as they apply to bosons before deriving the Hartree-Fock and random-phase-approximation (RPA) equations. In addition, I connect my approach to the Bogoliubov formulation for a system of interacting bosons and derive a configuration-interaction treatment. In Sec. III, I present a numerical method for solving the Hartree-Fock and RPA equations and in Sec. IV present results for the low-lying excitation frequencies of the JILA time orbiting potential trap [1,4].

II. THEORY

A. Review of second quantization

The notation of second quantization [15] simplifies the construction of properly symmetrized many-body states within the independent particle approximation. This simplification is especially useful for bosonic systems. A many-boson wave function is specified by the set of occupation numbers $\{n_\alpha\}$ where α represents all of the quantum numbers needed to label a single-particle state from some single-particle basis $\{\psi_\alpha(\mathbf{x})\}$. For instance,

$$|\Psi\rangle = |n_0,0,\ldots,0,n_i,0,\ldots\rangle \tag{1}$$

is a many-boson wave function with n_0 bosons in the 0th single-particle state, n_i bosons in the ith single-particle state, and no bosons in any other single-particle state. The sum of occupation numbers necessarily equals the total number of particles, i.e., $\Sigma_i n_i = N$. The above wave function may also be written as

$$|\Psi\rangle = \frac{(\hat{c}_0^\dagger)^{n_0}}{\sqrt{n_0!}}\frac{(\hat{c}_i^\dagger)^{n_i}}{\sqrt{n_i!}}|0\rangle.$$

Here, $|0\rangle$ is the state with no bosons present in any single-particle state. The creation, $\hat{c}_\alpha^\dagger$, and annihilation, $\hat{c}_\alpha$, operators create or annihilate a boson in the αth single-particle state in the following sense:

$$\hat{c}_\alpha^\dagger|\ldots,n_\alpha,\ldots\rangle = \sqrt{n_\alpha+1}|\ldots,n_\alpha+1,\ldots\rangle,$$

$$\hat{c}_\alpha|\ldots,n_\alpha,\ldots\rangle = \sqrt{n_\alpha}|\ldots,n_\alpha-1,\ldots\rangle.$$

Further, the $\hat{c}$'s satisfy the boson commutation relations

$$[\hat{c}_\alpha,\hat{c}_\beta^\dagger] = \delta_{\alpha\beta}, \quad \text{and } [\hat{c}_\alpha^\dagger,\hat{c}_\beta^\dagger] = [\hat{c}_\alpha,\hat{c}_\beta] = 0.$$

Yet another way to write the wave function in Eq. (1) is

$$\Psi_{n_0\cdots n_i\cdots}(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \mathcal{S}[\psi_0(\mathbf{x}_1)\cdots\psi_0(\mathbf{x}_{n_0})\psi_i(\mathbf{x}_{n_0+1})\cdots\psi_i(\mathbf{x}_N)],$$

where $\mathcal{S}$ is the symmetrization operator. This form explicitly makes the connection to the configuration space viewpoint more commonly adopted in the context of atomic-structure calculations.

B. Hartree-Fock approximation

With the Hartree-Fock approximation, one seeks the best independent particle wave function for a given set of occupation numbers. In the present case, I concentrate on the ground state of a system of bosons, i.e., $\{n_i\}=\{N,0,\ldots\}$; more general sets of occupation numbers can be used, however. Considerable freedom exists in the choice of a single-particle basis set. I use this flexibility to derive an equation for those single-particle states which minimize the total energy. Our derivation of the Hartree-Fock equation for bosons parallels standard Hartree-Fock derivations for fermions [15,18,19], so I outline only the essential steps. I begin with the second-quantized Hamiltonian

$$\hat{H}=\sum_{\alpha,\beta}\hat{c}^\dagger_\alpha\langle\alpha|H_0|\beta\rangle\hat{c}_\beta+\frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta}\hat{c}^\dagger_\alpha\hat{c}^\dagger_\beta\langle\alpha\beta|V|\gamma\delta\rangle\hat{c}_\delta\hat{c}_\gamma. \tag{2}$$

In this expression, all indices are summed over all single-particle states and

$$\langle\alpha|H_0|\beta\rangle=\int d^3x\,\psi^*_\alpha(\mathbf{x})H_0(\mathbf{x})\psi_\beta(\mathbf{x})$$

is the single-particle matrix element of

$$H_0(\mathbf{x})=-\frac{\hbar^2}{2m}\nabla^2+V_{\text{ext}}(\mathbf{x}),$$

which includes any external trapping potential in $V_{\text{ext}}(\mathbf{x})$. For example, in the present case $V_{\text{ext}}(\mathbf{x})$ is a cylindrically symmetric harmonic trapping potential; in atomic-structure calculations, $V_{\text{ext}}(\mathbf{x})$ is the electron-nucleus Coulomb interaction. The two-particle interaction matrix element in Eq. (2) is given by

$$\langle\alpha\beta|V|\gamma\delta\rangle=\int d^3x\int d^3x'\,\psi^*_\alpha(\mathbf{x})\psi^*_\beta(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')\times\psi_\gamma(\mathbf{x})\psi_\delta(\mathbf{x}').$$

For atoms in a trap $V(\mathbf{x})$ represents the interatomic potential while in atomic-structure calculations $V(\mathbf{x})$ describes the electron-electron Coulomb interaction. The $\psi_\alpha(\mathbf{x})$ in these matrix elements are the (as yet undetermined) single-particle orbitals which are orthonormal:

$$\int d^3x\,\psi^*_\alpha(\mathbf{x})\psi_\beta(\mathbf{x})=\delta_{\alpha\beta}.$$

To the extent that the potential energy of the system is described completely by a pairwise sum of two-body interactions and a sum of one-body trap potentials — which is my assumption throughout this paper — the Hamiltonian can be represented exactly by Eq. (2) for *any* choice of single-particle basis. Only when the composite nature of the particles is taken into account do three- or more-particle interactions enter. These multiparticle interactions, however, are typically weak and of much shorter range than the two-body interactions and are thus usually neglected.

To proceed, I solve the Schrödinger equation variationally using for a trial function the completely symmetric product wave function

$$\Phi(\mathbf{x}_1,\ldots,\mathbf{x}_N)=\phi(\mathbf{x}_1)\cdots\phi(\mathbf{x}_N). \tag{3}$$

The orbital $\phi(\mathbf{x})$ can, in turn, be expanded on a single-particle basis,

$$\phi(\mathbf{x})=\mathcal{N}\left[\psi_0(\mathbf{x})+\sum_{p\neq 0}^{\infty}a_p\psi_p(\mathbf{x})\right],$$

with $\mathcal{N}$ an overall normalization constant. I will choose the single-particle basis such that $\psi_0(\mathbf{x})$ alone is sufficient to minimize the total ground-state energy.

The first few terms in Eq. (3) are written in second quantization as

$$|\Phi\rangle=\mathcal{N}^N\left(1+\sum_{p\neq 0}a_p\frac{\hat{c}^\dagger_p\hat{c}_0}{\sqrt{N}}+\sum_{p,p'\neq 0}a_pa_{p'}\frac{\hat{c}^\dagger_p\hat{c}_0}{\sqrt{N-1}}\frac{\hat{c}^\dagger_{p'}\hat{c}_0}{\sqrt{N}}+\cdots\right)|\Phi_0^{\text{HF}}\rangle, \tag{4}$$

where $|\Phi_0^{\text{HF}}\rangle$ is the Hartree-Fock ground state of the system,

$$|\Phi_0^{\text{HF}}\rangle=\frac{(\hat{c}^\dagger_0)^N}{\sqrt{N!}}|0\rangle=|N,0,\ldots\rangle$$

or

$$\langle\mathbf{x}_1,\ldots,\mathbf{x}_N|\Phi_0^{\text{HF}}\rangle=\Phi_0^{\text{HF}}(\mathbf{x}_1,\ldots,\mathbf{x}_N)=\psi_0(\mathbf{x}_1)\cdots\psi_0(\mathbf{x}_N). \tag{5}$$

Thus the trial function includes multiple excitations of the Hartree-Fock ground state. Inasmuch as the ground energy eigenstate of the system of interacting bosons is the condensate, one can regard the Hartree-Fock ground state as a first approximation to the condensate wave function. It is only an approximation, however, since the true ground state of the system is a linear combination of the Hartree-Fock ground and excited states.

To determine the Hartree-Fock equation for $\psi_i(\mathbf{x})$, I require variations of the total energy E to be stationary with respect to single-particle excitations, which is equivalent to minimizing E with respect to the coefficients a_p,

$$\delta E=\frac{\delta}{\delta a_p}\left.\frac{\langle\Phi|\hat{H}|\Phi\rangle}{\langle\Phi|\Phi\rangle}\right|_{a_p=0}=0.$$

This leads to the condition

$$\left\langle \Phi_0^{\mathrm{HF}} \middle| \frac{\hat{c}_0^\dagger \hat{c}_p}{\sqrt{N}} \hat{H} \middle| \Phi_0^{\mathrm{HF}} \right\rangle = \langle \Phi_p^{\mathrm{HF}} | \hat{H} | \Phi_0^{\mathrm{HF}} \rangle = 0. \tag{6}$$

This condition ensures that the Hartree-Fock basis is chosen so that the Hamiltonian cannot produce single-particle excitations of $|\Phi_0^{\mathrm{HF}}\rangle$. Also, $|\Phi_0^{\mathrm{HF}}\rangle$ is variationally the best completely symmetric, single configuration, independent particle wave function just as the Hartree-Fock ground state for an atom is the best single Slater determinant wave function. In fact, an alternative method for deriving the Hartree-Fock equation for the ground state is to minimize the total energy with respect to $\psi_0(\mathbf{x})$. Equation (6) leads to the more general Hartree-Fock equation for the single-particle orbitals

$$H_0(\mathbf{x})\psi_i(\mathbf{x}) + \frac{N-1}{2}\left[\int d^3x'\, \psi_0^*(\mathbf{x}') V(\mathbf{x}-\mathbf{x}') \psi_0(\mathbf{x}') \psi_i(\mathbf{x}) + \int d^3x'\, \psi_0^*(\mathbf{x}') V(\mathbf{x}-\mathbf{x}') \psi_i(\mathbf{x}') \psi_0(\mathbf{x}) \right] = \varepsilon_i \psi_i(\mathbf{x}),$$

which holds for i including both the condensate and the excited orbitals. The first term in the square brackets is the direct contribution to the interaction energy and behaves as a local potential arising from the mean field due to the condensate, and the second term is the nonlocal exchange contribution to the interaction energy. Further, for a system of only one boson this reduces to the appropriate Schrödinger equation. For $i=0$ it simplifies such that the ground-state orbital $\psi_0(\mathbf{x})$ satisfies the analog of the nonlinear Schrödinger equation for the condensate wave function [see Refs. [15,20,21] and Eq. (28) below]

$$\left[H_0(\mathbf{x}) + (N-1) \int d^3x'\, \psi_0^*(\mathbf{x}') V(\mathbf{x}-\mathbf{x}') \psi_0(\mathbf{x}') \right] \psi_0(\mathbf{x}) = \varepsilon_0 \psi_0(\mathbf{x}). \tag{7}$$

The overall normalization of the Hartree-Fock ground state is ensured by normalizing $\psi_0(\mathbf{x})$ to unity.

The total energy of the condensate E_0^{HF} is not $N\varepsilon_0$ as might be expected but rather

$$E_0^{\mathrm{HF}} = \langle \Phi_0^{\mathrm{HF}} | \hat{H} | \Phi_0^{\mathrm{HF}} \rangle = N\varepsilon_0 - \frac{N(N-1)}{2} \langle 00|V|00\rangle. \tag{8}$$

The ''additional'' term can be understood as eliminating the double counting of pairs of particles included in $N\varepsilon_0$. In other words, $N\varepsilon_0$ includes the energy for each particle interacting with every other particle and so counts the contribution from a given pair twice as is familiar from electrostatics [22]. Similarly, the excitation energy in the Hartree-Fock approximation is not the difference of Hartree-Fock single-particle energies $\varepsilon_p - \varepsilon_0$, but rather

$$E_p^{\mathrm{HF}} - E_0^{\mathrm{HF}} = \langle \Phi_p^{\mathrm{HF}} | \hat{H} | \Phi_p^{\mathrm{HF}} \rangle - \langle \Phi_0^{\mathrm{HF}} | \hat{H} | \Phi_0^{\mathrm{HF}} \rangle \tag{9}$$

$$= (\varepsilon_p - \varepsilon_0) + \frac{N-1}{2} \langle p0|\overline{V}|p0\rangle. \tag{10}$$

In this expression, I have used the shorthand notation

$$\langle q0|\overline{V}|p0\rangle = \langle q0|V|p0\rangle + \langle q0|V|0p\rangle \tag{11}$$

for the direct and exchange contributions to the interparticle interaction matrix element. Note that the plus sign in this expression results from the requirement of symmetry upon permutation of the identical bosons (the requirement of antisymmetry for fermions yields a minus sign instead).

C. Random-phase approximation

I showed in Eq. (6) that the Hartree-Fock approximation accounts for single-particle excitations in the ground state. This approximation can be improved by including two- or more-particle excitations in the trial wave function. One approach that includes some of the physics of two-particle excitations is the random-phase approximation [15,18,19]. This method amounts to replacing the Hamiltonian, Eq. (2), by an effective Hamiltonian which accounts for up to two-particle excitations of the ground state. (The full Hamiltonian allows for single and double excitations of excited states as well.) The RPA equations or their equivalent can be derived in a number of ways. I will present a derivation based on the time-independent Schrödinger equation which makes the connection to the Bogoliubov approach most transparent. I could equivalently start from the time-dependent Schrödinger equation [18,19], or I could apply random-phase arguments [23] to linearize the interaction term in the Hamiltonian.

I begin with the exact solutions to the time-independent many-body Schrödinger equation,

$$\hat{H}|\nu\rangle = E_\nu |\nu\rangle,$$

and define operators $\hat{Q}_\nu$ such that

$$\hat{Q}_\nu |0\rangle = 0 \quad \text{and} \quad \hat{Q}_\nu^\dagger |0\rangle = |\nu\rangle,$$

where $|0\rangle$ is the exact many-body ground state. The energy of the νth excited state is written as

$$E_\nu = \frac{\langle \nu|\hat{H}|\nu\rangle}{\langle \nu|\nu\rangle}$$

or, using the properties of $\hat{Q}_\nu$, as

$$E_\nu - E_0 = \frac{\langle 0|[\hat{Q}_\nu,[\hat{H},\hat{Q}_\nu^\dagger]]|0\rangle}{\langle 0|[\hat{Q}_\nu,\hat{Q}_\nu^\dagger]|0\rangle}. \tag{12}$$

This is an equation for the energy difference—which is the experimentally measurable quantity—between the exact many-body excited state and the exact many-body ground state. One must, however, approximate the solution to Eq. (12). One approximation is the RPA [15,18,19], which consists of restricting $\hat{Q}$ to single-particle excitations,

$$\hat{Q}_\nu^\dagger = \frac{1}{\sqrt{N}} \sum_{p\neq 0} X_{p\nu} \hat{c}_p^\dagger \hat{c}_0 - Y_{p\nu} \hat{c}_0^\dagger \hat{c}_p, \tag{13}$$

where p refers to the Hartree-Fock single-particle basis. The first term removes a particle from the lowest Hartree-Fock orbital and places it in an excited orbital while the second term does the opposite. To consistently treat Eq. (12) in this approximation, both the eigenstates and eigenenergies must be approximated by their RPA equivalent. In particular, for $\hat{Q}$ defined by Eq. (13) I define the RPA ground state by

$$\hat{Q}_\nu|\Phi_0^{\rm RPA}\rangle=0$$

and the RPA excited states by

$$|\Phi_\nu^{\rm RPA}\rangle=\hat{Q}_\nu^\dagger|\Phi_0^{\rm RPA}\rangle.$$

With these definitions, the RPA version of Eq. (13) is written as

$$E_\nu^{\rm RPA}-E_0^{\rm RPA}=\frac{\langle\Phi_0^{\rm RPA}|[\hat{Q}_\nu,[\hat{H},\hat{Q}_\nu^\dagger]]|\Phi_0^{\rm RPA}\rangle}{\langle\Phi_0^{\rm RPA}|[\hat{Q}_\nu,\hat{Q}_\nu^\dagger]|\Phi_0^{\rm RPA}\rangle}. \tag{14}$$

This expression, like Eq. (12), would be an exact statement for the RPA quantities had it not been necessary to make the approximation $\hat{H}|\Phi_\nu^{\rm RPA}\rangle=E_\nu^{\rm RPA}|\Phi_\nu^{\rm RPA}\rangle$. Further, since the RPA ground state remains unknown, I make the approximation of replacing $|\Phi_0^{\rm RPA}\rangle$ by $|\Phi_0^{\rm HF}\rangle$ in order to evaluate the matrix elements in Eq. (14). With this replacement, the numerator of the right-hand side of Eq. (14) can be written as

$$\begin{aligned}\langle\Phi_0^{\rm HF}|[\hat{Q}_\nu,[\hat{H},\hat{Q}_\nu^\dagger]]|\Phi_0^{\rm HF}\rangle\\ &=\sum_{pp'\neq 0}X_{p\nu}^*[X_{p'\nu}B_{pp'}+Y_{p'\nu}C_{pp'}]\\ &\quad+Y_{p\nu}^*[X_{p'\nu}C_{pp'}^*+Y_{p'\nu}B_{pp'}^*],\end{aligned}$$

where

$$B_{pp'}=\frac{N-1}{2}\langle p0|\overline{V}|p'0\rangle+(\varepsilon_p-\varepsilon_0)\delta_{pp'},$$

$$C_{pp'}=\frac{N-1}{2}\langle pp'|\overline{V}|00\rangle. \tag{15}$$

Similarly, the denominator of the right-hand side of Eq. (14) can be written as

$$\langle\Phi_0^{\rm HF}|[\hat{Q}_\nu,\hat{Q}_\nu^\dagger]|\Phi_0^{\rm HF}\rangle=\sum_{p\neq 0}X_{p\nu}^*X_{p\nu}-Y_{p\nu}^*Y_{p\nu}.$$

Minimizing $E_\nu^{\rm RPA}$ in Eq. (14) with respect to $X_{q\nu}^*$ and $Y_{q\nu}^*$ yields the RPA equations

$$\sum_{p\neq 0}[X_{p\nu}B_{qp}+Y_{p\nu}C_{qp}]=\hbar\omega_\nu^{\rm RPA}X_{q\nu},$$

$$\sum_{p\neq 0}[X_{p\nu}C_{qp}^*+Y_{p\nu}B_{qp}^*]=-\hbar\omega_\nu^{\rm RPA}Y_{q\nu}, \tag{16}$$

where $\hbar\omega_{q0}=\varepsilon_q-\varepsilon_0$ and $\hbar\omega_\nu^{\rm RPA}=E_\nu^{\rm RPA}-E_0^{\rm RPA}$. I should emphasize that the RPA is *not* a variational approximation. In other words, the energies computed from Eq. (16) are not upper bounds to the true energies of the system. This property was lost when the matrix elements in Eq. (14) were evaluated only approximately. In addition, because of the minus sign in the second of the RPA equations, the excitation energies are not guaranteed to be real. It can be shown [18,19] that a complex energy indicates an instability of the Hartree-Fock solution. The stability of a condensate for negative scattering lengths could, for instance, be studied by searching for complex excitation energies as N is increased. The only differences between Eq. (16) and the RPA equations for fermions [15,18,19] are the factor of $(N-1)/2$ and the plus sign noted in Eq. (11) above.

The normalization of the eigenvectors of the RPA equations is determined by requiring the excited states to be orthonormal,

$$\langle\nu'|\nu\rangle=\langle\Phi_0^{\rm RPA}|[\hat{Q}_{\nu'},\hat{Q}_\nu^\dagger]|\Phi_0^{\rm RPA}\rangle=\delta_{\nu'\nu}. \tag{17}$$

But, approximating the RPA ground state by the Hartree-Fock ground state $|\Phi_0^{\rm HF}\rangle$ gives

$$\begin{aligned}\langle\Phi_0^{\rm RPA}|[\hat{Q}_{\nu'},\hat{Q}_\nu^\dagger]|\Phi_0^{\rm RPA}\rangle\\ &\approx\langle\Phi_0^{\rm HF}|[\hat{Q}_{\nu'},\hat{Q}_\nu^\dagger]|\Phi_0^{\rm HF}\rangle\\ &=\sum_{pp'\neq 0}(X_{\nu'p}^*X_{\nu p'}-Y_{\nu'p}^*Y_{\nu p'})\delta_{pp'}.\end{aligned} \tag{18}$$

Combined with Eq. (17) this gives the normalization condition

$$\sum_{p\neq 0}(X_{p\nu'}^*X_{p\nu}-Y_{p\nu'}^*Y_{p\nu})=\delta_{\nu'\nu}. \tag{19}$$

The substitution of the Hartree-Fock ground state for the RPA ground state is known as the quasiboson approximation [15,19]. It has been studied as an approximation to the interacting boson model in the study of nuclear structure [19]. In the nuclear structure problem, the interacting boson model replaces the pair of fermion operators which create a single-particle excitation of the ground state by an expansion on boson operators; the quasiboson approximation truncates this expansion to the first term. In the present problem, the quasiboson approximation replaces the pair of boson operators which create a single-particle excitation of the ground state by a single operator which also obeys boson commutation relations. That is, the quasiboson approximation effects the replacement

$$\frac{\hat{c}_p^\dagger\hat{c}_0}{\sqrt{N}}\rightarrow\hat{A}_p^\dagger.$$

The exact commutator is

$$\left[\frac{\hat{c}_0^\dagger\hat{c}_p}{\sqrt{N}},\frac{\hat{c}_{p'}^\dagger\hat{c}_0}{\sqrt{N}}\right]=\frac{\hat{c}_0^\dagger\hat{c}_0}{N}\delta_{pp'}-\frac{\hat{c}_{p'}^\dagger\hat{c}_p}{N}, \tag{20}$$

but the quasiboson approximation gives

$$[\hat{A}_p,\hat{A}_{p'}^\dagger]=\delta_{pp'}. \tag{21}$$

The relation of this replacement to the approximation of the RPA ground state by the Hartree-Fock ground state is made more clear by comparing the matrix elements of Eq. (20) and Eq. (21):

$$\frac{1}{N}\langle\Phi_0^{\mathrm{RPA}}|[\hat{c}_0^\dagger\hat{c}_p,\hat{c}_{p'}^\dagger\hat{c}_0]|\Phi_0^{\mathrm{RPA}}\rangle\approx\frac{1}{N}\langle\Phi_0^{\mathrm{HF}}|[\hat{c}_0^\dagger\hat{c}_p,\hat{c}_{p'}^\dagger\hat{c}_0]|\Phi_0^{\mathrm{HF}}\rangle$$

$$=\langle\Phi_0^{\mathrm{HF}}|[\hat{A}_p,\hat{A}_{p'}^\dagger]|\Phi_0^{\mathrm{HF}}\rangle=\delta_{pp'}.$$

The quasiboson approximation is thus valid only when the occupation of the Hartree-Fock excited states in the RPA ground state is small [15,19], and the error introduced in this case is on the order of N^{-1} due to the second term of the commutator in Eq. (20) above.

Within the quasiboson approximation, solving the RPA equations is equivalent to diagonalizing the quasiboson representation of the Hamiltonian $\hat{H}_B$ to second order in $\hat{A}$. $\hat{H}_B$ is defined by requiring that the matrix elements of the quasiboson representation operators be the same as the matrix elements of the corresponding operators in the original representation [19]. Explicitly, the definitions needed for the RPA are

$$\langle\Phi_0^{\mathrm{HF}}|\hat{H}_{\mathrm{B}}|\Phi_0^{\mathrm{HF}}\rangle=\langle\Phi_0^{\mathrm{HF}}|\hat{H}|\Phi_0^{\mathrm{HF}}\rangle=E_0^{\mathrm{HF}},$$

$$\langle\Phi_0^{\mathrm{HF}}|[\hat{A}_p,[\hat{H}_{\mathrm{B}},\hat{A}_{p'}^\dagger]]|\Phi_0^{\mathrm{HF}}\rangle$$

$$=\frac{1}{N}\langle\Phi_0^{\mathrm{HF}}|[\hat{c}_0^\dagger\hat{c}_p,[\hat{H},\hat{c}_{p'}^\dagger\hat{c}_0]]|\Phi_0^{\mathrm{HF}}\rangle=B_{pp'},$$

$$\langle\Phi_0^{\mathrm{HF}}|[\hat{A}_p,[\hat{H}_{\mathrm{B}},\hat{A}_{p'}]]|\Phi_0^{\mathrm{HF}}\rangle$$

$$=\frac{1}{N}\langle\Phi_0^{\mathrm{HF}}|[\hat{c}_0^\dagger\hat{c}_p,[\hat{H},\hat{c}_0^\dagger\hat{c}_{p'}]]|\Phi_0^{\mathrm{HF}}\rangle=-C_{pp'},$$

with $B_{pp'}$ and $C_{pp'}$ defined by Eq. (15). The quasiboson Hamiltonian is then written as

$$\hat{H}_B=E_0^{\mathrm{HF}}+\sum_{pp'\neq 0}B_{pp'}\hat{A}_p^\dagger\hat{A}_{p'}$$

$$+\frac{1}{2}\sum_{pp'\neq 0}C_{pp'}\hat{A}_p^\dagger\hat{A}_{p'}^\dagger+C_{pp'}^*\hat{A}_{p'}\hat{A}_p. \tag{22}$$

The terms linear in $\hat{A}$ and $\hat{A}^\dagger$ vanish identically by the Hartree-Fock condition, Eq. (6). Since it has a quadratic form, $\hat{H}_B$ can be diagonalized by a canonical (or Bogoliubov) transformation from the set of operators $\hat{A}$ to another set $\hat{O}$. In other words, I transform from the set of boson operators $\hat{A}$ for which the Hamiltonian is given by Eq. (22) and which satisfy

$$\hat{A}_p|\Phi_0^{\mathrm{HF}}\rangle=0 \quad \text{and} \quad \hat{A}_p^\dagger|\Phi_0^{\mathrm{HF}}\rangle=|\Phi_p^{\mathrm{HF}}\rangle$$

to a set $\hat{O}$ such that

$$\hat{O}_\nu|\Phi_0^{\mathrm{RPA}}\rangle=0 \quad \text{and} \quad \hat{O}_\nu^\dagger|\Phi_0^{\mathrm{RPA}}\rangle=|\Phi_\nu^{\mathrm{RPA}}\rangle.$$

The transformation which connects these two sets of operators is given by

$$\hat{O}_\nu^\dagger=\sum_{p\neq 0}X_{p\nu}\hat{A}_p^\dagger-Y_{p\nu}\hat{A}_p, \quad \hat{O}_\nu=\sum_{p\neq 0}X_{p\nu}^*\hat{A}_p-Y_{p\nu}^*\hat{A}_p^\dagger. \tag{23}$$

The operators $\hat{O}$ are the quasiboson approximations to the $\hat{Q}$ operators defined in Eq. (13). Further, for the transformation to be canonical, the $\hat{O}$'s must satisfy boson commutation relations just as the $\hat{A}$'s do. This requirement leads directly to the normalization condition Eq. (19) and places an additional constraint on the coefficients X and Y:

$$\sum_{p\neq 0}X_{p\nu'}Y_{p\nu}-X_{p\nu}Y_{p\nu'}=0.$$

In order to construct an approximate eigenstate within the RPA, the ground state must first be known. Using the Thouless theorem [24], the RPA ground state can be related to the Hartree-Fock ground state by

$$|\Phi_0^{\mathrm{RPA}}\rangle=\mathcal{N}e^{\hat{Z}}|\Phi_0^{\mathrm{HF}}\rangle.$$

In this expression, $\mathcal{N}$ is a normalization constant and

$$\hat{Z}=\frac{1}{2}\sum_{pp'\neq 0}Z_{pp'}\hat{A}_p^\dagger\hat{A}_{p'}^\dagger,$$

with the coefficient matrix $\mathbf{Z}$ given by

$$\mathbf{Z}^*=\mathbf{Y}\mathbf{X}^{-1}=\mathbf{Z}^\dagger.$$

Thus, because a product of two $\hat{A}^\dagger$'s is present in $\hat{Z}$, the exponential of $\hat{Z}$ will have only even powers of $\hat{A}^\dagger$. It follows that the RPA ground state contains only even numbers of particle excitations of the Hartree-Fock ground state. A direct calculation of the RPA ground state would then provide a means of checking the validity of the quasiboson approximation. If the coefficient $\mathcal{N}$ of the Hartree-Fock ground state in the expansion of the RPA ground state is near unity, then replacing the RPA ground state by the Hartree-Fock ground state is valid and the RPA ground state is a better approximation to the physical condensate. Conversely, if $\mathcal{N}$ is not nearly unity, the quasiboson RPA is not valid. In this case, a self-consistent RPA [19] might be used instead. That is, the RPA ground state calculated as described here could be used directly in Eq. (14) to derive new equations which could then be solved for a new set of X's and Y's. A new ground state could be calculated from these, and the procedure iterated until some convergence criterion is met.

Under the transformation Eq. (23) and taking into account the RPA equations (16), the Hamiltonian $\hat{H}_B$ becomes

$$\hat{H}_B=E_0^{\mathrm{RPA}}+\sum_{\nu\neq 0}\hbar\omega_\nu^{\mathrm{RPA}}\hat{O}_\nu^\dagger\hat{O}_\nu. \tag{24}$$

The total energy of the ground state in the RPA, E_0^{RPA}, can be related to the Hartree-Fock ground-state energy Eq. (8) by

$$E_0^{\mathrm{RPA}}=E_0^{\mathrm{HF}}-\sum_\nu\hbar\omega_\nu^{\mathrm{RPA}}\sum_{p\neq 0}|Y_{p\nu}|^2. \tag{25}$$

The RPA ground-state energy is lower than the Hartree-Fock energy, but as there is no variational bound on the RPA result, it can be lower than the true ground-state energy. In fact, it is not uncommon to find that this is the case for fermionic systems [19]; it results from the fact that the RPA can overestimate ground-state correlations.

I should point out that both the Hartree-Fock approximation and the RPA strictly conserve particle number. For the Hartree-Fock approximation, this follows from the fact that the number of particles is conserved in the Hartree-Fock equation, Eq. (7); and for the RPA, it can be seen that this is the case from the quasiboson Hamiltonian in Eq. (24). The $\hat{A}$ operators are defined to create single-particle excitations with the same total number of particles and so cannot change the total number of particles in any combination. This is in contrast to the Bogoliubov approximation in which the nonconservation of particle number leads to an overall shift of the absolute energies of the excitation spectrum [9].

D. Bogoliubov approximation

To better understand the differences and similarities between my formulation of the Hartree-Fock approximation and the RPA for bosons and the Bogoliubov approach more commonly used for boson systems, I reproduce here the basics of the Bogoliubov derivation for a general two-body interaction. The essence of the Bogoliubov approximation lies in treating the condensate (i.e., the ground state) separately from the rest of the system based on the relative occupation of the condensate versus excited states. The assumption is that the condensate has on the order of N particles while the excited states collectively have on the order of 1 particle. Having made this approximation, an effective Hamiltonian is derived which has a quadratic dependence on excitation — or fluctuation — operators just as in the RPA. This quadratic form can be diagonalized through the use of a canonical transformation [15] as was used for the quasiboson Hamiltonian $\hat{H}_B$. I begin with the following form for the Hamiltonian [15]:

$$\hat{H}=\int d^3x\,\hat{\psi}^\dagger(\mathbf{x})H_0(\mathbf{x})\hat{\psi}(\mathbf{x})+\frac{1}{2}\int d^3x\int d^3x'\,\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{x}'). \tag{26}$$

This can be obtained from Eq. (2) provided the field operator $\hat{\psi}(\mathbf{x})$ $[\hat{\psi}^\dagger(\mathbf{x})]$ is given by

$$\hat{\psi}(\mathbf{x})=\sum_\alpha \phi_\alpha(\mathbf{x})\hat{c}_\alpha,$$

where $\hat{c}$ $(\hat{c}^\dagger)$ is as before and $\phi_\alpha(\mathbf{x})$ is an undetermined single-particle state that need not be from the set $\{\psi_\alpha(\mathbf{x})\}$ used in the previous two sections. In fact, I will show that they are similar but not identical to the Hartree-Fock orbitals. The standard Bogoliubov approach [15] separates the condensate from the excited states in the field operator (and its adjoint),

$$\hat{\psi}(\mathbf{x})=\phi_0(\mathbf{x})\hat{c}_0+\sum_{\alpha\neq 0}\phi_\alpha(\mathbf{x})\hat{c}_\alpha,$$

replaces the operators $\hat{c}_0$ $(\hat{c}_0^\dagger)$ by the c number $\sqrt{N_0}$, and collects the sum over excited states into a fluctuation operator $\hat{\varphi}(\mathbf{x})$ $[\hat{\varphi}^\dagger(\mathbf{x})]$,

$$\hat{\varphi}(\mathbf{x})=\sum_{\alpha\neq 0}\phi_\alpha(\mathbf{x})\hat{c}_\alpha.$$

Physically, this operator annihilates (creates) a particle in a singly excited state at position $\mathbf{x}$ and must be small, in some sense, compared to the condensate wave function in order to justify the expansion of the Hamiltonian only through quadratic terms. This condition for the validity of the Bogoliubov effective Hamiltonian is the equivalent of the quasiboson approximation discussed for the RPA. The total field operator is then just

$$\hat{\psi}(\mathbf{x})=\sqrt{N_0}\phi_0(\mathbf{x})+\hat{\varphi}(\mathbf{x}). \tag{27}$$

The consequence of this replacement is that the number operator

$$\begin{aligned}\hat{N}&=\int d^3x\,\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\\&=N_0+\sqrt{N_0}\int d^3x[\phi_0^*(\mathbf{x})\hat{\varphi}(\mathbf{x})+\hat{\varphi}^\dagger(\mathbf{x})\phi_0(\mathbf{x})]\\&\quad+\int d^3x\,\hat{\varphi}^\dagger(\mathbf{x})\hat{\varphi}(\mathbf{x})\end{aligned}$$

no longer commutes with the Hamiltonian so that the number of particles is not conserved. This shortcoming can be approximately overcome by instead using the grand canonical Hamiltonian, $\hat{K}=\hat{H}-\mu\hat{N}$ [15]. In this expression, μ is the chemical potential which will be used at a later point to fix the average number of particles. Excitation energies can be computed directly within this approach, but it has recently been pointed out [9] that the fact that the number of particles is not conserved implies the existence of a spurious solution of the normal-mode equations with a vanishing excitation energy. With the field operator from Eq. (27) substituted into $\hat{K}$ and terms through $O(\hat{\varphi}^2)$ retained, $\hat{K}$ can be diagonalized with the canonical transformation [7,15]

$$\hat{\varphi}(\mathbf{x})=\sum_\lambda u_\lambda(\mathbf{x})\hat{\beta}_\lambda+v_\lambda^*(\mathbf{x})\hat{\beta}_\lambda^\dagger.$$

The $\hat{\beta}_\lambda$ $(\hat{\beta}_\lambda^\dagger)$ are interpreted as annihilation (creation) operators for quasiparticles. Diagonalizing $\hat{K}$ in this approximation is thus equivalent to transforming to a system of noninteracting quasiparticles [see Eq. (24)]. $\hat{K}$ can only be diagonalized, however, provided the condensate wave function $\phi_0(\mathbf{x})$ satisfies the self-consistent equation

$$\left[H_0(\mathbf{x})+N_0\int d^3x'\,\phi_0^*(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')\phi_0(\mathbf{x}')\right]\phi_0(\mathbf{x})=\mu\phi_0(\mathbf{x}). \tag{28}$$

This condition eliminates terms linear in $\hat{\varphi}(\mathbf{x})$ from $\hat{K}$ and is known as the nonlinear Schrödinger equation or the Ginzburg-Pitaevskii-Gross equation [20]. Given the interpretation of $\hat{\varphi}(\mathbf{x})$, it is evident that this condition builds single-particle excitations into the condensate wave function in basically the same way as the Hartree-Fock condition builds them into the Hartree-Fock ground state. It is thus the equivalent of the Hartree-Fock equation, Eq. (7), obtained in Sec. II B. Further, just as the RPA included only single and double excitations, keeping terms through $O(\hat{\varphi}^2)$ in $\hat{K}$ allows only single and double excitations of the condensate wave function.

The grand canonical Hamiltonian takes the simple form

$$\hat{K}=E_0-\mu N_0-\sum_{\lambda}\hbar\Omega_\lambda\int d^3x v_\lambda^*(\mathbf{x})v_\lambda(\mathbf{x})+\sum_{\lambda}\hbar\Omega_\lambda\hat{\beta}_\lambda^\dagger\hat{\beta}_\lambda \tag{29}$$

provided $u_\lambda(\mathbf{x})$ and $v_\lambda(\mathbf{x})$ satisfy the normal-mode equations

$$\begin{aligned}&\left[H_0(\mathbf{x})-\mu+N_0\int d^3x'\,\phi_0^*(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')\phi_0(\mathbf{x}')\right]u_\lambda(\mathbf{x})\\&\quad+N_0\int d^3x'\,\phi_0^*(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')u_\lambda(\mathbf{x}')\phi_0(\mathbf{x})\\&\quad+N_0\int d^3x'\,\phi_0(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')v_\lambda(\mathbf{x}')\phi_0(\mathbf{x})\\&=\hbar\Omega_\lambda u_\lambda(\mathbf{x}),\end{aligned}\tag{30}$$

$$\begin{aligned}&\left[H_0(\mathbf{x})-\mu+N_0\int d^3x'\,\phi_0^*(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')\phi_0(\mathbf{x}')\right]v_\lambda(\mathbf{x})\\&\quad+N_0\int d^3x'\,\phi_0(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')v_\lambda(\mathbf{x}')\phi_0^*(\mathbf{x})\\&\quad+N_0\int d^3x'\,\phi_0^*(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')u_\lambda(\mathbf{x}')\phi_0^*(\mathbf{x})\\&=-\hbar\Omega_\lambda v_\lambda(\mathbf{x}).\end{aligned}\tag{31}$$

In these equations, $\hbar\Omega_\lambda$ is the excitation energy, and the solutions $u_\lambda(\mathbf{x})$ and $v_\lambda(\mathbf{x})$ are normalized as

$$\int d^3x u_{\lambda'}^*(\mathbf{x})u_\lambda(\mathbf{x})-v_{\lambda'}^*(\mathbf{x})v_\lambda(\mathbf{x})=\delta_{\lambda'\lambda}.$$

In order to relate the Bogoliubov normal-mode equations to the RPA equations, I expand $u_\lambda(\mathbf{x})$ and $v_\lambda(\mathbf{x})$ on the set of single-particle states which satisfy the equation

$$\begin{aligned}&H_0(\mathbf{x})\phi_i(\mathbf{x})+\frac{N_0}{2}\left[\int d^3x'\,\phi_0^*(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')\phi_0(\mathbf{x}')\phi_i(\mathbf{x})\right.\\&\quad\left.+\int d^3x'\,\phi_0^*(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')\phi_i(\mathbf{x}')\phi_0(\mathbf{x})\right]=\epsilon_i\phi_i(\mathbf{x}),\end{aligned}$$

where $\epsilon_0=\mu$. Note that this equation is chosen in analogy to the Hartree-Fock equation rather than derived within the Bogoliubov approximation. However, this basis is physically sensible as it includes the mean-field effects of the condensate. Using such a basis to solve the normal-mode equations would most likely require fewer — possibly far fewer — states than would be needed if $u_\lambda(\mathbf{x})$ and $v_\lambda(\mathbf{x})$ were expanded in terms of a harmonic oscillator basis. Writing the expansions as

$$u_\lambda(\mathbf{x})=\sum_{p\neq0}U_{\lambda p}\phi_p(\mathbf{x}),$$

$$v_\lambda(\mathbf{x})=\sum_{p\neq0}V_{\lambda p}\phi_p(\mathbf{x})$$

and assuming the $\phi_i(\mathbf{x})$ to be real, I have

$$\begin{aligned}&\frac{N_0}{2}\sum_{p\neq0}[U_{\lambda p}\langle q0|\overline{V}|p0\rangle+V_{\lambda p}\langle qp|\overline{V}|00\rangle]+(\epsilon_q-\mu)U_{\lambda q}\\&\quad=\hbar\Omega_\lambda U_{\lambda q},\\&\frac{N_0}{2}\sum_{p\neq0}[U_{\lambda p}\langle qp|\overline{V}|00\rangle+V_{\lambda p}\langle q0|\overline{V}|p0\rangle]+(\epsilon_q-\mu)V_{\lambda q}\\&\quad=-\hbar\Omega_\lambda V_{\lambda q}.\end{aligned}\tag{32}$$

These equations are very similar to the RPA equations; the only difference in form is the presence of N_0 rather than $N-1$. For large N and low-lying excitations, this difference is negligible considering the order N^{-1} errors already introduced at various points in each approximation. However, there is also a more subtle difference. Where the Hartree-Fock single-particle basis functions strictly conserve particle number, the single-particle basis functions to which the labels refer in Eq. (32) have built into them the order N^{-1} error present in the nonlinear Schrödinger equation, Eq. (28). The most significant difference, then, between the Bogoliubov approximation and the RPA is the exclusion of terms of order N^{-1} from the self-consistent ground state in the Bogoliubov approximation and the consequent loss of particle number conservation. In the RPA, both the quasiboson and the exact (within the RPA) ground state conserve particle number.

The shift in the ground-state energy from Eq. (29) when written in the $\{\phi_i(\mathbf{x})\}$ representation has the same form as Eq. (25),

$$\sum_{\lambda}\hbar\Omega_\lambda\int d^3x v_\lambda^*(\mathbf{x})v_\lambda(\mathbf{x})=\sum_{\lambda}\hbar\Omega_\lambda\sum_{p\neq0}|V_{\lambda p}|^2. \tag{33}$$

The spurious mode of Lewenstein and You [9] leads to an additional shift of the ground state. Since this shift results from particle nonconservation in the condensate wave function, the total shift of the ground-state energy — Eq. (33) plus the spurious mode shift — should be equal to the RPA ground-state energy shift Eq. (25) since the number of particles is strictly conserved in the Hartree-Fock ground state giving no spurious mode solution to the RPA equations. With Eq. (33) substituted, the grand canonical Hamiltonian Eq. (29) looks very much like the RPA effective Hamiltonian Eq. (24). In the RPA effective Hamiltonian there is, of course, no chemical potential term, and the RPA equivalent of the quasiparticle operators $\hat{\beta}$ are the $\hat{O}$ operators in Eq. (23).

E. Configuration interaction

A connection to standard atomic-structure methods can be made by applying configuration interaction (CI) [17] to the system of bosons. The term configuration in this context means a given set of occupation numbers $\{n_i\}$ corresponding to the set of single-particle orbitals $\{\psi_i(\mathbf{x})\}$ defined in Sec. II B. Configuration interaction, then, is the variational approach in which the trial wave function is expanded on a complete basis of many-body wave functions — or configurations — including the condensate and singly to multiply excited configurations. Since this is a complete many-body basis, the exact, time-independent, many-body energy eigenstates can in principle be calculated. In practice, of course, one must limit the expansion to a finite number of basis functions.

Explicitly, I assume a trial wave function of the form

$$|\Psi\rangle = a_0|N,0,\ldots\rangle + \sum_{p\neq 0} a_p|N-1,0,\ldots,0,1_p,0,\ldots\rangle + \sum_{p,p'\neq 0} b_{pp'}|N-2,0,\ldots,0,1_p,0,\ldots,0,1_{p'},0,\ldots\rangle + \cdots, \tag{34}$$

where the notation 1_p indicates that the pth Hartree-Fock orbital is occupied by one boson. This trial function includes the same basis functions as Eq. (4), the trial function used to derive the Hartree-Fock equation, but it is not constrained to be a product form. Specifically, the coefficients for multiple excitations do not factor into products as they did in Eq. (4). This wave function is thus the most general completely symmetric wave function as opposed to the most general completely symmetric *product* wave function. Upon truncation, the variational principle for the total energy yields the matrix eigenvalue problem

$$\mathbf{H}\Psi_\nu = E_\nu \Psi_\nu,$$

where Ψ_ν is the vector of expansion coefficients. Since neither the RPA nor the Bogoliubov equations are variational approximations, one cannot expect to ''derive'' them from CI. To obtain a similar approximation, however, it is only necessary to include up to doubly excited configurations [that is, truncate the trial function $|\Psi\rangle$ to those terms explicitly written in Eq. (34)]. It is possible to go beyond the RPA and the Bogoliubov approximation within the CI framework with the inclusion of triple and higher excitations. In fact, the inclusion of all double excitation matrix elements, i.e., those that involve one- and two-particle excitations of *excited* states as well as the ground state, improves upon both the RPA and the Bogoliubov approximations. This improvement stems from the fact that CI is a variational approximation based upon an expansion on a complete set of states, and the inclusion of higher and more varied excitations not included in the RPA or the Bogoliubov approximation must yield better approximations to the exact energy eigenstates. Physically, this improvement can be described as incorporating correlations beyond both the RPA and the Bogoliubov approximation.

The Hamiltonian matrix in this truncated space can then be partitioned into submatrices according to the states that are coupled: the ground state G, singly excited states S, or doubly excited states D. Explicitly,

$$\mathbf{H} = \begin{pmatrix} H_{GG} & H_{GS} & H_{GD} \\ H_{SG} & H_{SS} & H_{SD} \\ H_{DG} & H_{DS} & H_{DD} \end{pmatrix}.$$

For example, the submatrix $H_{GS}=H_{SG}^{\mathrm{T}}$ contains the coupling between the ground state and singly excited states. For Hartree-Fock single-particle orbitals, all of the elements of this submatrix are identically zero by the Hartree-Fock condition, Eq. (6). The full CI matrix equation is then

$$\begin{pmatrix} H_{GG} & 0 & H_{GD} \\ 0 & H_{SS} & H_{SD} \\ H_{DG} & H_{DS} & H_{DD} \end{pmatrix} \begin{pmatrix} a_G \\ a_S \\ b_D \end{pmatrix}_\nu = E_\nu \begin{pmatrix} a_G \\ a_S \\ b_D \end{pmatrix}_\nu , \tag{35}$$

with E_ν the total energy of the νth state. In order to connect this set of equations as closely as possible to the RPA and Bogoliubov equations, recall that in both the RPA and Bogoliubov approaches only those matrix elements coupling single-particle excitations to single-particle excitations and two-particle excitations to the ground state are retained. Keeping only these matrix elements in the CI matrix, or equivalently keeping terms proportional to N^2 and N while neglecting terms proportional to $\sqrt{N}$ and 1 results in setting H_{SD} and H_{DS} to zero and approximating H_{DD} by H'_{DD}. The RPA-like approximation to CI reads

$$\begin{pmatrix} H_{GG} & 0 & H_{GD} \\ 0 & H_{SS} & 0 \\ H_{DS} & 0 & H'_{DD} \end{pmatrix} \begin{pmatrix} a_G \\ a_S \\ b_D \end{pmatrix}_\nu = E_\nu \begin{pmatrix} a_G \\ a_S \\ b_D \end{pmatrix}_\nu . \tag{36}$$

In this approximation, single excitations are decoupled from double excitations as well as from the ground state. Because the submatrices decouple, I can permute the rows and columns to bring $\mathbf{H}$ to block diagonal form and diagonalize within the subspace of single-particle excitations separately to find the low-lying excited state energies,

$$H_{SS}a_S^\nu = E_\nu a_S^\nu. \tag{37}$$

Diagonalizing the remainder of the matrix gives corrections to the ground state and higher-lying excited states. H_{SS} can be evaluated explicitly:

$$(H_{SS})_{qp} = E_0^{\mathrm{HF}}\delta_{qp} + B_{qp},$$

with B_{qp} from Eq. (15). Substituted in Eq. (37), this gives after rearranging

$$Ba_S^\nu = \hbar\omega_\nu^{\mathrm{TDA}} a_S^\nu.$$

This is a special case of the RPA equations with $Y_{q\nu}$ set to zero and $X_{q\nu}$ replaced by a_S^ν. It is, in fact, the Tamm-Dancoff approximation (TDA) [15,18,19] which, unlike the RPA, *is* variational (with the constraint that the ground state is the Hartree-Fock ground state). This is readily understood since it is just a more severely truncated ($b_{pp'}=0$) CI expansion.

So, while I have evaluated the CI Hamiltonian in Eq. (36) to the same order in N as the RPA, the RPA-like CI spectrum is presumably less accurate than the RPA spectrum since the coupling between single and double excitations is neglected. However, with the further modifications $a_0 \rightarrow 1$ and $b_{pp'} \rightarrow a_p a_{p'}$, the CI equation (36) becomes qualitatively more like the RPA equations: the submatrix H_{GG} drops out; H_{GD}, H_{SS}, and H_{DG} become coupled; and H_{DD} is neglected as it is then of order a_p^4 (in other words, it includes terms like two-particle excitations of excited states which are neglected in the RPA). This approach does [18,19], in fact, lead to a set of equations much like the RPA equations, Eq. (16). These are usually derived in the context of stability analysis for the Hartree-Fock ground state. This interpretation comes from the fact that the equations describe the quadratic behavior of the multidimensional energy surface in ''a_p space'' near a minimum. The surface is quadratic in this approximation because the highest excitations allowed are two-particle excitations of the ground state which are proportional to a_p^2 [see Eq. (4)]. The condition for locating the minimum in this space is just the Hartree-Fock condition itself. However, the minimum thus found is almost certainly not a global minimum (except in the unlikely event that the Hartree-Fock solution is the exact solution), but rather a constrained minimum. Thus negative eigenvalues of these equations correspond to a negative curvature of the energy surface or, equivalently, an unstable equilibrium. The Hartree-Fock solution in this case is only an extremum in the energy, not a minimum, and so does not describe the ground state of the system.

III. NUMERICAL METHOD

For an arbitrary interparticle potential, it is necessary to solve the Hartree-Fock and RPA equations numerically. I turn now to a numerical method for solving these equations. Consider a system of atoms trapped by a cylindrically symmetric harmonic potential; this is the applicable symmetry for the traps at JILA [1,4], at Rice [2], and at MIT [3,5]. Since I am interested in the ground state and in low-lying excited states for which the de Broglie wavelengths are much larger than the range of the interparticle potential $V(\mathbf{x}-\mathbf{x}')$, I assume that it can be approximated as

$$V(\mathbf{x}-\mathbf{x}')=\frac{4\pi\hbar^2 a_{\rm sc}}{M}\,\delta(\mathbf{x}-\mathbf{x}'), \tag{38}$$

with $a_{\rm sc}$ the s-wave scattering length and M the atomic mass. In the language of many-body perturbation theory, using the true scattering length $a_{\rm sc}$ rather than the Born approximation to the scattering length,

$$a_{\rm B}=\frac{M}{4\pi\hbar^2}\int d^3x V(\mathbf{x}),$$

is effectively the same as summing the ladder diagrams which can, in turn, be thought of as summing the Born series for the scattering amplitude. In order to account for two-body collision energies different from zero, I could use for the interparticle interaction the configuration space scattering T matrix instead of a δ function [18]. However, the energy dependence of the T matrix over the energy range of importance should be negligible. Physically, replacing $a_{\rm B}$ by $a_{\rm sc}$ accounts for multiple interactions between two particles and is critical in cases where the interaction potential has a strongly repulsive core [15,25]. I have also assumed that the average interparticle spacing is much larger than $a_{\rm sc}$ so that the effects of other particles can be neglected in obtaining the effective two-body interaction. This assumption is typically stated as $na_{\rm sc}^3 \ll 1$ where n is a characteristic number density in the trap. The use of Eq. (38) has also been justified from the viewpoint that it is the first term of a pseudopotential expansion [18,26] which is constructed so as to reproduce the low-energy s-wave scattering phase shift.

With a δ-function interaction and a harmonic trapping potential, the Hartree-Fock equation, Eq. (7), simplifies to

$$\begin{aligned}\Bigg[-\frac{\hbar^2}{2M}\nabla^2+\frac{1}{2}M(\omega_\rho^2\rho^2+\omega_z^2z^2)\\ +\frac{4\pi\hbar^2a_{\rm sc}}{M}(N-1)|\psi_0(\rho,\phi,z)|^2\Bigg]\psi_i(\rho,\phi,z)\\ =\varepsilon_i\psi_i(\rho,\phi,z).\end{aligned} \tag{39}$$

I assume that the single-particle orbitals have the same symmetries as the trapping potential. Specifically, I take them to be eigenstates of L_z and Π_z which are the projection of orbital angular momentum on the z axis and the parity with respect to the xy plane, respectively. Each single-particle orbital is thus labeled by an energy quantum number n and the quantum numbers m and π_z for L_z and Π_z, respectively. These symmetry considerations lead to the following choice for $\psi_i(\mathbf{x})$:

$$\psi_i(\rho,\phi,z)=\beta^{-3/2}\chi_{n|m|}^{\pi_z}(\xi,\eta)\frac{e^{im\phi}}{\sqrt{2\pi}}.$$

In this expression, β is the length scale for a harmonic oscillator of frequency ω,

$$\beta=\sqrt{\frac{\hbar}{M\omega}}.$$

The scaled coordinates ξ and η are related to the physical coordinates by

$$\rho=\beta\xi \quad \text{and} \quad z=\beta\eta.$$

The specific form of $\psi_i(\mathbf{x})$ is chosen so that

$$\int \xi d\xi \int d\eta|\chi_i(\xi,\eta)|^2=1$$

gives

$$\int \rho d\rho \int dz \int d\phi|\psi_i(\rho,z,\phi)|^2=1.$$

The rescaled Hartree-Fock equation for $\chi_i(\xi,\eta)$ now reads

$$\left[-\frac{1}{2\xi}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial}{\partial\xi}\right)-\frac{1}{2}\frac{\partial^2}{\partial\eta^2}+\frac{m^2}{2\xi^2}+\frac{1}{2}(\omega_\xi^2\xi^2+\omega_\eta^2\eta^2)+2\alpha|\chi_0(\xi,\eta)|^2\right]\chi_i(\xi,\eta)=\tilde{\varepsilon}_i\chi_i(\xi,\eta), \tag{40}$$

where the dimensionless trap freqencies are $\omega_\xi=\omega_\rho/\omega$, $\omega_\eta=\omega_z/\omega$, the scaled single-particle energy is $\tilde{\varepsilon}_i=\varepsilon_i/\hbar\omega$, and the dimensionless nonlinear parameter that characterizes the interaction strength is

$$\alpha=(N-1)\frac{a_{\mathrm{sc}}}{\beta}.$$

From Eq. (40) one can show that all energies with $m>0$ are doubly degenerate. For the ground state, Eq. (40) is a self-consistent equation which I solve iteratively [17] using two-dimensional (2D) finite elements [27]. That is, I solve Eq. (40) using a guess for the mean-field contribution to the potential and iterate until the energy has converged to within some tolerance. In the present case, I require the relative tolerance from one iteration to the next to be no more than 10^{-8}. The guess for the ith iteration is given by

$$\chi_0^i(\xi,\eta)=(1-\gamma)\chi_0^{i-2}(\xi,\eta)+\gamma\chi_0^{i-1}(\xi,\eta),$$

with $0.05\leqslant\gamma\leqslant0.5$. This iteration can stall for a few to several steps without converging further, or can fail altogether to converge for γ too large. This difficulty is overcome by making an adaptive reduction of γ as the solution is iterated. For small values of the nonlinear parameter α, I use the harmonic oscillator ground state as the initial guess and begin the iteration with larger values of γ, while for large values of α I use the Thomas-Fermi solution [28] and begin with smaller values of γ. One advantage of the iterative approach over other techniques of solving the self-consistent equation [7,21] is that the solution for a given α is obtained directly without the need to renormalize. Having obtained the self-consistent ground state, it becomes straightforward to solve for the excited orbitals, since the equation is then a linear Schrödinger equation with a static potential comprised of the trapping potential plus the mean-field contribution of the condensate. The resulting set of single-particle orbitals thus forms a complete, orthonormal basis.

Now that a set of single-particle orbitals has been determined, I can set up and solve the RPA equations. To do this, I first need the interaction matrix elements. As in Eq. (39), for δ-function interactions the direct and exchange contributions to the potential matrix elements are indentical. In other words, $\langle q0|V|p0\rangle=\langle q0|V|0p\rangle$. With $p\equiv\{n,m,\pi_z\}$,

$$\langle p'0|V|p0\rangle=\frac{2\hbar^2 a_{\mathrm{sc}}}{M\beta^3}\mathcal{V}_{p'0,p0},$$

with the dimensionless matrix element defined by

$$\mathcal{V}_{p'0,p0}=\delta_{m,m'}\delta_{\pi_z,\pi_z'}V_{p'p}, \tag{41}$$

where

$$V_{p'p}=\int\xi d\xi\int d\eta\chi_{n'|m|}^{\pi_z}(\xi,\eta)|\chi_{00}^{+}(\xi,\eta)|^2\chi_{n|m|}^{\pi_z}(\xi,\eta).$$

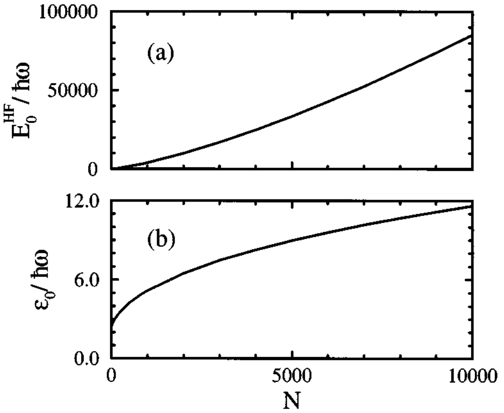

FIG. 1. For ^{87}Rb atoms and the JILA TOP trap parameters, the (a) total Hartree-Fock ground-state energy E_0^{HF} and (b) Hartree-Fock ground-state orbital energy ε_0 as a function of particle number scaled by the frequency $\omega=\omega_\rho$.

In the same notation,

$$\mathcal{V}_{p'p,00}=\delta_{m,-m'}\delta_{\pi_z,\pi_z'}V_{p'p}. \tag{42}$$

The only difference between the matrix elements in Eqs. (41) and (42) — the δ function in m — arises physically from conservation of total L_z. Thus only states with the same total projection M_L are coupled. The parity δ function is also readily understood since both matrix elements are integrated over all z and contain χ_0^2, which is an even function of z. The RPA equations then reduce to

$$\begin{pmatrix}\tilde{B} & \tilde{C}\\ \tilde{C} & \tilde{B}\end{pmatrix}\begin{pmatrix}X\\ Y\end{pmatrix}=\tilde{\omega}\begin{pmatrix}I & 0\\ 0 & -I\end{pmatrix}\begin{pmatrix}X\\ Y\end{pmatrix}, \tag{43}$$

where $\tilde{\omega}_\nu/\omega$ is the rescaled excitation frequency and

$$\tilde{B}_{qp}=2\alpha\mathcal{V}_{q0,p0}+\tilde{\omega}_{q0}\delta_{qp},$$

$$\tilde{C}_{qp}=2\alpha\mathcal{V}_{qp,00}$$

are the rescaled matrices from Eq. (15).

The δ functions in the expressions for the integrals reduce the computational burden of solving the RPA equations significantly. Specifically, the RPA equations can be diagonalized separately for each π_z and $|m|$. Moreover, the structure of the RPA matrix yields automatically that all excitation energies for each positive m are degenerate with the excitation energies for $-m$.

IV. RESULTS AND DISCUSSION

I have solved the Hartree-Fock and RPA equations for parameters appropriate to the JILA experiment, $\nu_\rho=\nu_z/\sqrt{8}=133$ Hz [1,4] and $a_{\mathrm{sc}}=110$ a.u. [29]. Note that in all of my numerical calculations I choose the frequency scale ω to be ω_ρ. I show in Fig. 1 the Hartree-Fock energies for the ground state as a function of the number N of trapped atoms. In Fig. 1(a), I plot the total Hartree-Fock ground-state energy

E_0^{HF} from Eq. (8); and in Fig. 1(b), the Hartree-Fock ground-state orbital energy ε_0. The N dependence of the two is quite different as is, of course, their physical interpretation. The total energy in Fig. 1(a) sets the absolute scale for the excitation spectrum while the orbital energy is the energy necessary to remove one atom completely from the condensate. For $N=5000$, I have also calculated the RPA shift in the ground-state energy $\Delta E_0=|E_0^{\mathrm{RPA}}-E_0^{\mathrm{HF}}|$ to be $162.10\hbar\omega$. This lowers the Hartree-Fock ground-state energy of $33\,492\hbar\omega$ by only 0.5% which is a good indication that the quasiboson approximation, replacing the RPA ground state by the Hartree-Fock ground state, is valid.

From the expression for the RPA ground-state energy, Eq. (25), the excitation spectrum and transformation coefficients for all m and π_z must in principle be calculated in order to evaluate the ground-state energy shift. To approximately compute the energy shift, however, I solved the RPA equations for $m\leqslant 10$ and both z parities, constructed the scaled sum

$$\Delta\widetilde{E}_0^{m\pi_z}=\sum_{\nu}\widetilde{\omega}_\nu|Y_{m\pi_z\nu}|^2,$$

and extrapolated $\Delta\widetilde{E}_0^{m\pi_z}$ to $m\to\infty$ using the empirical expression

$$\Delta\widetilde{E}_0^{m\pi_z}=\widetilde{\epsilon}_{\pi_z}e^{-\delta_{\pi_z}m}.$$

This form fit the calculated points quite well over an order of magnitude decrease in $\Delta\widetilde{E}_0^{m\pi_z}$ between $m=0$ and $m=10$ for both parities. Including the degeneracy in m, the full ground-state shift is then

$$\Delta\widetilde{E}_0=\sum_{\pi_z}\left(\Delta\widetilde{E}_0^{0\pi_z}+2\sum_{m=1}^{10}\Delta\widetilde{E}_0^{m\pi_z}+2\widetilde{\epsilon}_{\pi_z}\sum_{m=11}^{\infty}e^{-\delta_{\pi_z}m}\right).$$

The last sum over m involves a geometric series and is thus easily evaluated. I find that when summed over both parities it contributes approximately 14% to the total energy shift. It follows that the errors introduced through the empirical fit will lead to only small errors in the total energy shift.

To solve the RPA equations, it is only necessary to include a small number of Hartree-Fock single-particle orbitals in order to obtain few percent accuracies in the low-lying excitation energies. For example, with $N=5000$ atoms and $m=0$, a basis set of ten Hartree-Fock orbitals gives the lowest excitation energy to an accuracy of 0.7% compared to the converged result. In Table I, I show the convergence behavior for the lowest five excitation energies for $N=5000$ and $m=0$. When 60 orbitals are used, for instance, the lowest excitation energy is converged to six significant figures. For comparison, I can estimate the number of harmonic oscillator states necessary to obtain the same convergence by expanding the highest-energy Hartree-Fock orbital in terms of harmonic oscillator states. Restricting the harmonic oscillator expansion using both m and π_z, i.e., including only $n_x=n_y$ and even n_z, I find that it takes approximately 80 oscillator states to represent the 60th Hartree-Fock orbital. I should point out, however, that the comparison for $m=0$ is the most favorable to the oscillator expansion since nonzero m will require about twice as many oscillator states as for $m=0$. In addition, as the nonlinear parameter α increases, the number of oscillator states needed to achieve a given level of convergence increases whereas the number of Hartree-Fock orbitals remains essentially constant.

TABLE I. The convergence of the RPA spectrum with respect to the size of the Hartree-Fock single-particle orbital basis for $N=5000$ ^{87}Rb atoms and the JILA trap parameters. The frequencies $\widetilde{\omega}_\nu$ are the scaled frequencies ω_ν/ω.

N_{basis}	$\widetilde{\omega}_1$	$\widetilde{\omega}_2$	$\widetilde{\omega}_3$	$\widetilde{\omega}_4$	$\widetilde{\omega}_5$
10	1.87193	3.29129	4.77010	5.50449	6.21153
20	1.86003	3.26675	4.71695	5.15355	5.98377
40	1.85963	3.26573	4.71530	5.14483	5.97368
60	1.85958	3.26562	4.71512	5.14438	5.97331
80	1.85958	3.26562	4.71510	5.14432	5.97322

In order to better understand whether excited-state and ground-state correlations make significant contributions to the excitation spectrum, I have calculated the spectrum in three of the approximations discussed above: the Hartree-Fock approximation, the Tamm-Dancoff approximation, and the random-phase approximation. The Hartree-Fock approximation includes no correlation beyond those implied by identical particle statistics. All of the Hartree-Fock many-body states are thus simply symmetrized product states, or single configurations. The TDA is based upon an expansion on Hartree-Fock single-particle orbitals and allows correlations only among the singly excited Hartree-Fock states. In other words, the TDA excited states are linear combinations of the Hartree-Fock singly excited states. The ground state in the TDA, however, is just the Hartree-Fock ground state. The RPA improves upon TDA by allowing correlations in the ground state as well as the excited states. So, in the RPA both the ground state and the excited states will be linear combinations of the Hartree-Fock ground and excited states.

I show in Figs. 2–4 the results of these calculations for both z parities and $m=0$, 1, and 2. I expect that the RPA spectrum should be the most accurate of the three approximations as it includes the most correlation among the Hartree-Fock states. Given this expectation, one sees from Figs. 2(a)–2(c) that the Hartree-Fock excitation spectrum [calculated from $\hbar\omega_\nu^{\mathrm{HF}}=E_p^{\mathrm{HF}}-E_0^{\mathrm{HF}}$ and Eq. (10)] is in rea-

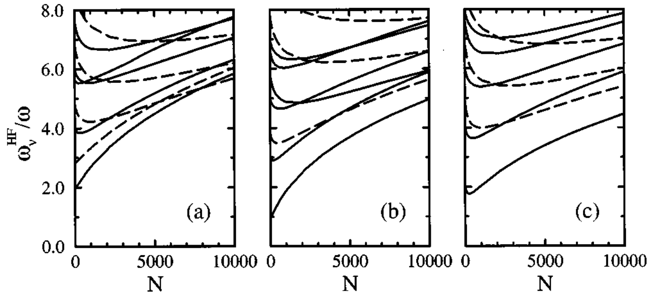

FIG. 2. The lowest frequencies of the Hartree-Fock approximation to the excitation spectrum for ^{87}Rb atoms in the JILA TOP trap scaled by the frequency $\omega=\omega_\rho$. (a) $m=0$, (b) $m=1$, and (c) $m=2$. In each graph solid lines are even z parity and dashed lines are odd z parity.

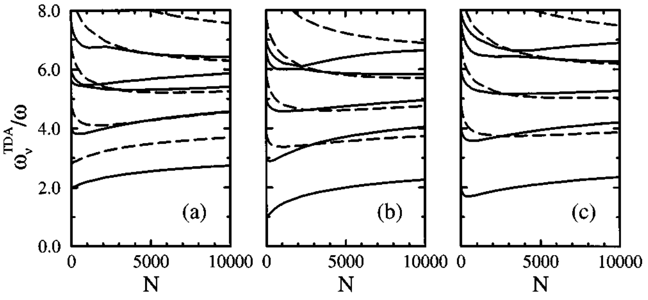

FIG. 3. The lowest frequencies of the Tamm-Dancoff approximation to the excitation spectrum for ^{87}Rb atoms in the JILA TOP trap scaled by the frequency $\omega=\omega_\rho$. (a) $m=0$, (b) $m=1$, and (c) $m=2$. In each graph solid lines are even z parity and dashed lines are odd z parity.

sonable agreement with the RPA energies only for the higher-lying states for N less than a few hundred to a thousand. This agreement suggests that the excitation is adequately described by the simple picture of a single particle being excited out of the ground state to a higher-lying Hartree-Fock state. Arguing on the basis of the nodal structure of the single-particle orbitals and Eq. (10), the agreement for higher-lying excitations and odd z parity seems reasonable since the mean field due to the condensate has less overlap with higher-lying excited states which have an increasing number of nodes in the region of the mean field. Since the difference in Hartree-Fock single-particle orbital energies, $\varepsilon_p-\varepsilon_0$, decreases as N increases due to the flattening and widening of the bottom of the harmonic trapping potential by the mean field, the overlap of the single-particle orbital and the mean field must be responsible for the increase in the Hartree-Fock excitation energies with increasing N [see Eq. (10)]. By a similar argument, odd z-parity states will have less overlap with the condensate mean field than even z-parity states with a similar energy since they have a node at $z=0$ rather than an antinode. This is also the reason that the Hartree-Fock spectrum for odd z-parity states is qualitatively closer to the RPA spectrum for larger N than the even z-parity states.

The TDA spectrum in Figs. 3(a)–3(c) is an improvement on the Hartree-Fock spectrum although the close agreement with the RPA spectrum is over essentially the same region of small N. However, for larger N the TDA spectrum is quite a large improvement over the Hartree-Fock spectrum. I conclude that excited-state correlations are important, but that the ground-state correlations included in the RPA calculation are essential for accurate excitation energies. In Figs. 4(a)–4(c) I show the RPA excitation spectrum along with the experimental points from the recent JILA measurement [4]. The agreement of the experimental points with the RPA spectrum—and disagreement with the other two spectra—bears out the expectation that the RPA is the more accurate approximation. However, the agreement is not perfect as I show in Fig. 5. Further, as shown in Ref. [4], the agreement of the RPA spectrum with the excitation spectrum obtained by Edwards *et al.* [6] from the Bogoliubov approximation is quite good over the range of N they computed.

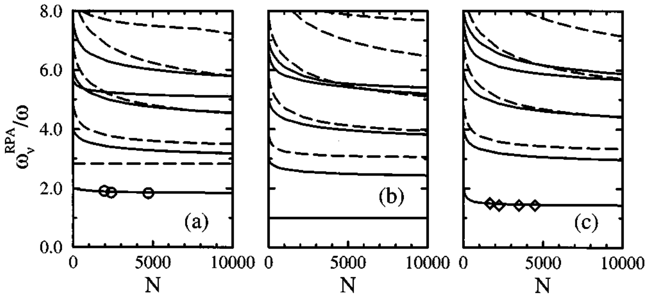

FIG. 4. The lowest frequencies of the random-phase approximation to the excitation spectrum for ^{87}Rb atoms in the JILA TOP trap scaled by the frequency $\omega=\omega_\rho$. (a) $m=0$, (b) $m=1$, and (c) $m=2$. In each graph, solid lines are even z parity and dashed lines are odd z parity. Also shown are the JILA experimental measurements.

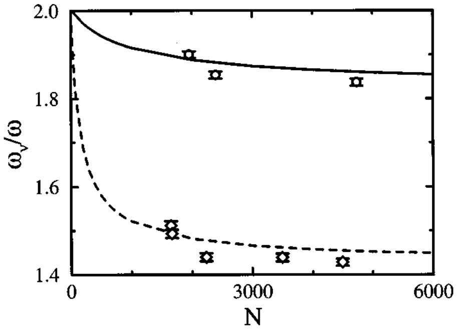

FIG. 5. Comparison of the lowest $m=0$ (solid line) and $m=2$ (dashed line) random-phase-approximation excitation frequencies with the JILA experimental measurements.

V. SUMMARY

I have modified the Hartree-Fock, random-phase, and configuration-interaction approximations for use with systems of interacting bosons and have shown that they can be treated accurately and efficiently within particle number conserving approximations. In fact, I make approximations which are remarkably similar to those made in the standard Bogoliubov approach and derive largely the same equations while maintaining particle number conservation. I have also shown that systems of interacting bosons can be treated in a manner analogous to that used to describe the electronic states of atoms. This allows me to adapt the knowledge and intuition gained from the atomic-structure problem to understand the quantum mechanical states of interacting, trapped atoms.

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[1] M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, and E.A. Cornell, Science **269**, 198 (1995).

[2] C.C. Bradley, C.A. Sackett, J.J. Tollett, and R.G. Hulet, Phys. Rev. Lett. **75**, 1687 (1995); R.G. Hulet, C.C. Bradley, C.A. Sackett, and J.J. Tollett, Bull. Am. Phys. Soc. **41**, 1130 (1996).

[3] K.B. Davis, M.O. Mewes, M.R. Andrews, N.J. van Druten, D.D. Durfee, D.M. Kim, and W. Ketterle, Phys. Rev. Lett. **75**, 3969 (1995).

[4] D.S. Jin, J.R. Ensher, M.R. Matthews, C.E. Wieman, and E.A. Cornell, Phys. Rev. Lett. **77**, 420 (1996).

[5] M.O. Mewes, M.R. Andrews, N.J. van Druten, D.M. Kurn, D.S. Durfee, C.G. Townsend, and W. Ketterle, Phys. Rev. Lett. **77**, 988 (1996).

[6] M. Edwards, P.A. Ruprecht, K. Burnett, R.J. Dodd, and C.W. Clark, Phys. Rev. Lett. **77**, 1671 (1996).

[7] M. Edwards, P.A. Ruprecht, K. Burnett, and C.W. Clark, Phys. Rev. A **54**, 4178 (1996).

[8] L. You, W. Hoston, M. Lewenstein, and K. Huang (unpublished).

[9] M. Lewenstein and L. You, Phys. Rev. Lett. **77**, 3489 (1996).

[10] S. Stringari, Phys. Rev. Lett. **77**, 2360 (1996).

[11] W.C. Wu and A. Griffin, Phys. Rev. A **54**, 4204 (1996).

[12] M. Marinescu and A.F. Starace (unpublished).

[13] K.G. Singh and D.S. Rokhsar, Phys. Rev. Lett. **77**, 1667 (1996).

[14] A.L. Fetter, Phys. Rev. A **53**, 4245 (1996).

[15] A.L. Fetter and J.D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).

[16] B.D. Esry and C.H. Greene, Bull. Am. Phys. Soc. **41**, 1137 (1996).

[17] R.D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981), Chap. 13.

[18] A. deShalit and H. Feshbach, *Theoretical Nuclear Physics Volume 1: Nuclear Structure* (Wiley, New York, 1974).

[19] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer, New York, 1980).

[20] V.L. Ginzburg and L.P. Pitaevskii, Zh. Éksp. Teor. Fiz. **34**, 1240 (1958) [Sov. Phys. JETP **7**, 858 (1958)]; E.P. Gross, J. Math. Phys. **4**, 195 (1963).

[21] M. Edwards and K. Burnett, Phys. Rev. A **51**, 1382 (1995).

[22] J.D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1975), p. 45.

[23] D. Bohm and D. Pines, Phys. Rev. **92**, 609 (1953).

[24] D.J. Thouless, Nucl. Phys. **21**, 225 (1960).

[25] B.D. Esry and C.H. Greene (unpublished).

[26] K. Huang, *Statistical Mechanics* (Wiley, New York, 1963); K. Huang and C.N. Yang, Phys. Rev. **105**, 767 (1957).

[27] Y. Zhou, C.D. Lin, and J. Shertzer, J. Phys. B **26**, 3937 (1993).

[28] F. Dalfovo and S. Stringari, Phys. Rev. A **53**, 2477 (1996).

[29] H.M.J.M. Boesten, C.C. Tsai, J.R. Gardner, D.J. Heinzen, and B.J. Verhaar, Phys. Rev. A (to be published).