Exact many-body wave function and properties of trapped bosons in the infinite-particle limit

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The emphasis of this work is on the computation of physical properties as well as of the wave function of interacting bosons in a trap potential. Many-body perturbation theory is employed to study the leading term of these quantities for finite numbers of bosons, and exact solutions are aimed at in the infinite-particle limit. As discussed before, a suitable starting point is the second-quantized Hamiltonian represented in the basis of destruction and creation operators of its own mean-field potential. This choice leads to expressions for the perturbation terms of all quantities which exhibit a very weak dependence on the particle number. Importantly, when applying ideas similar to Bogoliubov's, the Hamiltonian can be reduced in the infinite-particle limit to a much simplified form which is *a priori* particle-number conserving. The resulting phonon Hamiltonian is diagonalizable by a linear transformation for which an explicit eigenvalue equation is given. Physical properties can be expressed explicitly by elements of this transformation, and of particular relevance is that the particle-number-conserving wave functions of the original many-boson system can be reconstructed using recursion relations. The reconstruction of the particle-conserving wave function from the phonon Hamiltonian can also be used to assess when the infinite-particle limit is reached in practice for finite trapped condensates. Two applications are discussed in detail. For one of them, an exact solution is known which is found, in the infinite-particle limit, to exactly coincide with that of the phonon Hamiltonian. In both examples expressions for the properties are given in closed form. The physics behind the phonon Hamiltonian and its physical properties is discussed.

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I. INTRODUCTION

Many-body theory has been widely and successfully used for decades to investigate nuclei [1,2], solids [3,4], atoms, molecules, and clusters [5–8]. In contrast, there have only been a few attempts to study systems made of bosons using such theory mainly because Wick's theorem cannot be utilized to expand the relevant physical quantities in Goldstone or Feynman diagrams [3]. Nevertheless, some typical and successful methods of electronic structure have been reformulated for bosons, such as the configuration interaction and random phase approximations [9], coupled-cluster theory [10,11], and many-body perturbation theory [12], which are useful also for bosons.

On the other hand, systems made of identical bosons can condense and form Bose-Einstein condensates (BECs), which, in contrast to fermions, are amenable to simplified theoretical descriptions, in particular, in the infinite-particle limit. Since the experimental discovery of BECs consisting of dilute atomic gases in a trap potential [13–15], there has been enormous interest in their properties [16–18]. Here, the Gross-Pitaevskii (GP) equation [19,20] has played a leading role. This equation is obtained by minimizing the Gross-Pitaevskii energy functional [9,21] and is a mean-field equation. Its simplicity and the facts that it can be solved rather straightforwardly and exhibits many interesting and appealing properties have added much to its popularity. Importantly, it has been rigorously proven by Lieb and Seiringer (LS theorem) [22] that under some conditions (see below) the GP equation provides in the infinite-particle limit the exact energy and density per particle as does the full many-particle Schrödinger equation. One immediate and highly relevant consequence of this proof is that BECs are 100% condensed in this limit. In this limit, also called the GP or mean-field limit, the interaction parameter $\Lambda = \lambda_0(N-1)$ appearing in the GP equation, where λ_0 is the two-particle interaction strength, is kept fixed as the number of particles $N \to \infty$.

Recently, it has been demonstrated that in spite of the fact that the GP equation provides in the infinite-particle limit the exact energy and density per particle, the overlap of the GP and of the exact many-boson wave functions is always smaller than 1 and can be very small and even vanish [12]. There, it has also been shown that the exact wave function is usually rather complex and gives rise to substantial correlation between the bosons not included in the GP equation. That such correlations can be relevant has also been discussed in [23–26]. Moreover, the proof of the LS theorem mentioned above is restricted to 3 and 2 dimensions and, in addition, assumes the existence of a finite scattering length, but it could be shown that the result of the theorem applies also for cases not covered by the available proof, i.e., to 1 dimension and to cases where a finite scattering length does not exist [12].

In free space, i.e., in the absence of a trap, it is known that the GP ground-state wave function exhibits inconsistencies [3,17]. These inconsistencies are removed by the theory of Bogoliubov, where in the full Hamiltonian of the system only the terms leading in N are retained [3,27]. The calculation is performed for the thermodynamic limit of the homogeneous system and it is assumed that the depletion of the condensate is small. This theory is not number conserving and has been extended to become a number-conserving Bogoliubov theory by Girardeau [28] and by Gardiner [29]. Fetter [30] has formulated a non-particle-conserving Bogoliubov theory for spatially inhomogeneous gases, i.e., gases in a trap potential,

and this theory has been extended by Gardiner [29] to be a particle-conserving one. In inhomogeneous trapped systems the thermodynamic limit is not the relevant limit and one resorts to the infinite-particle limit discussed above where $N \to \infty$ while the interaction parameter $\Lambda = \lambda_0(N-1)$ is kept fixed [22]. For completeness we mention that there have been successful attempts to formulate the theory of Bogoliubov in a mathematically rigorous way; see [31–35] and references therein.

In the present work we aim at solving the many-body problem of bosons in a trap in the infinite-particle limit. Our starting point is also based on the idea of Bogoliubov, namely that for large N nearly all bosons are in the condensed part of the system and one has only to discuss the fluctuations of the system. As mentioned above, the mean-field theory has been found to yield the exact density per particle in the infinite-particle limit, implying that the depletion per particle indeed vanishes. We thus base our theory on the full Hamiltonian expressed in the basis of creation and annihilation operators defined by the mean-field Hamiltonian. While this idea is not new [9,10,12], we shall see that it can be taken further than previously attempted. Here, we mention that we follow the definition of mean-field given by Leggett [17] and many others, where the many-body wave function is given by the Hartree ansatz, i.e., a simple product of single-particle functions with no two-particle or higher correlations, and is just a particular case of the Hartree-Fock-Bogoliubov approximation; see [36]. The full Hamiltonian is written as a sum of the mean-field Hamiltonian, which becomes the unperturbed Hamiltonian, and a perturbation describing the fluctuations beyond the mean-field. We shall show that the theory formulated in this manner is *a priori* particle-number conserving. The former works on Bogoliubov theory have been formulated for contact interaction $V(\mathbf{r}_i - \mathbf{r}_j) = \delta(\mathbf{r}_i - \mathbf{r}_j)$ between the bosons. Here, as also done in [9,10,12], we formulate our theory for a general two-body interaction potential $V(\mathbf{r}_i - \mathbf{r}_j)$. Apart for being more general, we would like to mention that a contact potential has no meaning in many-body theory in three and two dimensions (3D and 2D for brevity). It has been demonstrated that as the bosons can avoid each other in 2D and 3D in the presence of contact interaction, the exact solution in these dimensions gives identical results to those if there is no interaction at all [37–39].

Here, we shall discuss, apart from the general theory, several quantities of interest, such as the boson correlation energy, the overlap of the exact wave function and of the mean-field wave function, the reduced density matrix, and the depletion of the condensate. This is done in the framework of perturbation theory for the general case of N bosons, as well as exactly for the infinite-particle limit. It will also be shown that in the infinite-particle limit not only the fluctuations of the condensate, but, in principle, also the complete wave function can be reconstructed from the theory. This is particularly relevant, as the wave function determines all physical quantities of the system. As already mentioned above, the exact wave function can be extremely different from the mean-field wave function [12]. Explicit examples will also be shown.

As the number of trapped particles in a given trap potential is increased keeping Λ fixed, the density increases and one may wonder about the connection of the infinite-particle limit to cold-atom experiments where the gases used are dilute. This problem is resolved by noticing that the results obtained for physical quantities (and even for the wave function) in the infinite-particle limit also apply for finite numbers of bosons. From our analytical and numerical findings we may conclude that for a given trap potential there is a large range of interaction strengths where the results obtained in the infinite-particle limit also apply for finite numbers of bosons as used in typical cold-atom experiments.

We would like to mention that it is not possible to apply the results obtained for a system in a trap to the homogenous case in the thermodynamic limit. This issue is discussed in some detail by Lieb and Seiringer [22]. In brief, as is well known for the homogeneous case in the thermodynamic limit, the BEC has a depleted fraction even in the ground state. In contrast, BEC in a trap is 100% condensed in the infinite-particle limit; i.e., the depletion per particle vanishes for infinitely many particles. The two limits, the thermodynamic and mean-field limits, are not the same and cannot be interchanged.

The paper is organized as follows. In Sec. II the leading term in the perturbation expansion of the properties of interest and of the wave function is derived for arbitrary values of N. Section III is devoted to the reduction of the Hamiltonian and the derivation of its properties in the infinite-particle limit. There, the reconstruction of the particle-number-conserving wave function in the infinite-particle limit is also discussed. Two applications are presented in Secs. IV and V, where the properties and wave functions are computed in the infinite-particle limit and compared with known exact results whenever available and with the results of the perturbation theory.

II. THE GENERAL HAMILTONIAN AND ITS PROPERTIES

A. The mean field as the unperturbed Hamiltonian

In this short subsection we would like to express the Hamiltonian for bosons using the creation and destruction operators of the mean-field potential as usually done in electronic structure theory. As already mentioned in the introduction, this has already been proposed before [9,10,12]. The Hamiltonian of N identical bosons in a trap potential interacting by a two-particle potential reads

$$H = \sum_{i=1}^{N} h(\mathbf{r}_i) + \sum_{j>i} \lambda_0 V(\mathbf{r}_i - \mathbf{r}_j). \tag{1}$$

Here, $h(\mathbf{r})$ is the one-body Hamiltonian comprising the kinetic energy of a boson and its trap potential, and λ_0 is the strength of the interaction between the bosons. Minimizing the expectation value of H taken with the mean-field ansatz $\varphi_0(\mathbf{r_1})\varphi_0(\mathbf{r_2})\ldots\varphi_0(\mathbf{r_N})$, where all bosons reside in a one-particle state φ_0, also called orbital, one obtains the mean-field equation for this orbital:

$$[h + v]\varphi_0(\mathbf{r}) = \mu_0\varphi_0(\mathbf{r}), \tag{2}$$

$$v = \Lambda \int \left|\varphi_0(\mathbf{r}')\right|^2 V(\mathbf{r} - \mathbf{r}')d\mathbf{r}'.$$

The quantity μ_0 is the (mean-field) chemical potential, and v is the mean-field potential. In the case of contact interaction,

the latter becomes $v = \Lambda|\varphi_0(\mathbf{r})|^2$ and is usually called the GP potential, and φ_0 the GP one-particle state.

The above equation defines a Fock-like operator $\hat{F}$ which has a complete set of orthonormal solutions φ_i with eigenvalues μ_i, with $= 0,1,2,\ldots$, and is rewritten to give

$$\hat{F}\varphi_i(\mathbf{r}) = \mu_i\varphi_i(\mathbf{r}),$$
$$\hat{F} = h + v. \tag{3}$$

We can now simply add in Eq. (1) the mean-field potential v to the one-particle Hamiltonian h and subtract it again from the two-body interaction potential and rewrite this equation to take on the form

$$H = H_0 + \lambda_0 W, \tag{4}$$

where $H_0 = \sum_{j=1}^{N} \hat{F}(\mathbf{r}_j)$ is now the unperturbed Hamiltonian and $\lambda_0 W = \lambda_0 V - v$ is the residual interaction. This interaction describes the fluctuations beyond mean field.

For convenience, we now transfer the above equation, Eq. (4), to second quantization by introducing as usual the boson creation operators $b_i^\dagger$ corresponding to the solutions $\varphi_i(\mathbf{r})$. Then, the Hamiltonian takes on the following appearance:

$$H = \sum_{i=1}^{N} \mu_i b_i^\dagger b_i + \left[\frac{\lambda_0}{2}\sum_{i,j,k,l} V_{ijkl} b_i^\dagger b_j^\dagger b_l b_k - \Lambda \sum_{i,k} V_{i0k0} b_i^\dagger b_k\right]. \tag{5}$$

The first term of H is the second quantized representation of H_0 and the term in brackets that of the interaction potential $\lambda_0 W$. The matrix elements V_{ijkl} appearing in the Hamiltonian read, as usual,

$$V_{ijkl} = \int \varphi_i^*(\mathbf{r})\varphi_j^*(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\varphi_k(\mathbf{r})\varphi_l(\mathbf{r}')d\mathbf{r}d\mathbf{r}'.$$

It is seen that for interactions which depend on the distance between two bosons, $V_{ijkl} = V_{jilk} = V_{klij}^* = V_{lkji}^*$, and for real orbitals one has the additional symmetry $V_{ijkl} = V_{kjil} = V_{ilkj}$.

The orthonormal eigenstates of the unperturbed, i.e., mean-field, Hamiltonian H_0 can all be cast into the simple form

$$|q_0,q_1,\ldots,q_m\rangle = \frac{(b_0^\dagger)^{q_0}(b_1^\dagger)^{q_1}\cdots(b_m^\dagger)^{q_m}}{\sqrt{q_0!q_1!\cdots q_m!}}|\mathrm{vac}\rangle. \tag{6}$$

Here and thereafter $|\mathrm{vac}\rangle$ is the boson vacuum, and the total number of bosons $q_0 + q_1 + \ldots + q_m = N$ is conserved. The ground mean-field state of the N bosons is just $|\mathrm{MF}\rangle = |N\rangle = [N!]^{-1/2}(b_0^\dagger)^N|0\rangle$. Note that zero occupations $q_i = 0$ are not indicated in the eigenstates. It is easily seen that

$$H_0|q_0,\ldots,q_m\rangle = \left[\sum_i \mu_i q_i\right]|q_0,\ldots,q_m\rangle, \tag{7}$$

and, in particular, $H_0|N\rangle = N\mu_0|N\rangle$.

Finally, we mention that the general rules to evaluate matrix elements of operators in the basis of the Fock states Eq. (6) can be found in [40].

B. Many-body perturbation theory in terms of Λ

Having separated the Hamiltonian into the unperturbed Hamiltonian and the residual interaction, we can perform a many-body perturbation theory [12] for any boson number N, where the parameter of the perturbation is Λ. We shall use this theory to give *new explicit expressions* for the leading terms in the expansion of Λ of properties relevant to this work. These expressions are of interest by themselves as they reflect the physics of the properties, but they will also serve as a stringent test for applications of our main theory to be developed in the next section. We shall see below that using the mean field as the unperturbed Hamiltonian gives rise to a particularly appealing behavior of the properties.

In perturbation theory the eigenstate $|\tilde{\Psi}\rangle$ in the intermediate normalization $\langle\tilde{\Psi}^{(0)}|\tilde{\Psi}\rangle = 1$, where $|\tilde{\Psi}^{(0)}\rangle$ is the normalized unperturbed state, is expanded in orders of the perturbation parameter [8]. In our case, the expansion is in orders of Λ and $|\tilde{\Psi}^{(0)}\rangle = |N\rangle$. For that purpose one defines a projector $\hat{Q} = 1 - |N\rangle\langle N|$ which removes the unperturbed state from all the terms $|\tilde{\Psi}^{(n)}\rangle$, $n > 0$ of the expansion. The expansion can be cast in a compact form:

$$|\tilde{\Psi}\rangle = \sum_{n=0} |\tilde{\Psi}^{(n)}\rangle,$$
$$|\tilde{\Psi}^{(n)}\rangle = \left\{\frac{\hat{Q}}{N\mu_0 - H_0}(\lambda_0 W - \Delta E)\right\}^n |N\rangle. \tag{8}$$

Here, $\Delta E = E_{\mathrm{exact}} - N\mu_0$ is the energy difference between that of the exact and the unperturbed state. Employing the expansion of the state in Eq. (8), one obtains the expansion of this quantity as well:

$$\Delta E = \sum_{n=1} E^{(n)},$$
$$E^{(n)} = \langle N|\lambda_0 W|\tilde{\Psi}^{(n-1)}\rangle. \tag{9}$$

As usual, the unperturbed energy is $E^{(0)} = \langle N|H_0|N\rangle$ and the sum of the zeroth- and first-order energies $E^{(0)} + E^{(1)}$ is the mean-field energy $E_{\mathrm{MF}} = \langle N|H|N\rangle$, i.e., the expectation value of the Hamiltonian taken with the unperturbed state. In our case, the mean-field energy takes on the appearance

$$E_{\mathrm{MF}} = N\mu_0 - \frac{N\Lambda}{2}V_{0000},$$

where the matrix element V_{0000} is defined below Eq. (5).

As a last remark we mention that the exact normalized state is, of course, given by $|\Psi_{\mathrm{exact}}\rangle = |\tilde{\Psi}\rangle/\langle\tilde{\Psi}|\tilde{\Psi}\rangle^{1/2}$.

C. Relevant physical properties and their leading term in Λ

In this subsection several physical quantities relevant to our work are introduced and briefly discussed, generally and also in the light of the perturbation theory of the preceding subsection as well as for large boson numbers N.

1. The wave function

The Fock states introduced in Eq. (6) are the eigenstates of the mean-field operator and form a complete orthonormal set. As usual, any exact eigenstate $|\Psi\rangle$ of the Hamiltonian H can

be expanded in this set:

$$|\Psi\rangle = \sum C_{\vec{q}}|\vec{q}\rangle.$$

In perturbation theory, the coefficients $C_{\vec{q}}$ are determined by the expansion in Eq. (8). In zeroth order one has $|N\rangle$ and in first order one has to evaluate the quantity $\lambda_0 W|N\rangle$. As $\lambda_0 W = \lambda_0 V - v$, we first operate with $\lambda_0 V$ and obtain

$$\begin{aligned}\lambda_0 V|N\rangle &= \frac{\lambda_0}{2}\sum_{i,j,k,l} V_{ijkl} b_i^\dagger b_j^\dagger b_l b_k |N\rangle \\ &= \lambda_0\sqrt{N(N-1)}\Bigg\{\sum_i \sqrt{N-1}V_{i000}|N-1,1_i\rangle \\ &\quad + \frac{1}{\sqrt{2}}\sum_i V_{ii00}|N-2,2_i\rangle \\ &\quad + \frac{1}{2}\sum_{i,j} V_{ij00}|N-2,1_i,1_j\rangle\Bigg\}.\end{aligned}$$

Remembering that the interaction strength $\Lambda = \lambda_0(N-1)$ is held fixed, we see that the first term in the above equation is proportional to $\sqrt{N}$ while the other two do not depend on the number of bosons for large N. This makes the expansion problematic for large N. However, applying the mean-field potential gives

$$\begin{aligned}-\Lambda v|N\rangle &= -\Lambda\sum_{i,k} V_{i0k0} b_i^\dagger b_k |N\rangle \\ &= -\Lambda\sqrt{N}\sum_i V_{i000}|N-1,1_i\rangle,\end{aligned}$$

which compensates the original term proportional to $\sqrt{N}$ exactly. The first-order correction to the wave function thus reads

$$\begin{aligned}|\tilde{\Psi}^{(1)}\rangle = \Lambda\sqrt{\frac{N}{(N-1)}}\Bigg\{&\frac{1}{\sqrt{2}}\sum_i \frac{V_{ii00}}{2\mu_0 - 2\mu_i}|N-2,2_i\rangle \\ &+\frac{1}{2}\sum_{i,j}\frac{V_{ij00}}{2\mu_0-\mu_i-\mu_j}|N-2,1_i,1_j\rangle\Bigg\}. \quad (10)\end{aligned}$$

All terms are now independent of N for large boson numbers, underlining the relevance of choosing the mean-field as the unperturbed Hamiltonian. The above expression for the first-order wave function is needed to compute the leading correction for small Λ of all the properties discussed below.

2. *The overlap of the mean-field and exact wave functions*

The overlap $S(N) = \langle N|\Psi\rangle$ between the exact and mean-field wave functions is a straightforward and relevant measure for the quality of the mean-field wave function. Knowing that the mean-field energy and density per particle are exact in the infinite-particle limit [12,22] makes the analysis of the exact wave function particularly important because this wave function determines all physical quantities beyond mean field.

This overlap is simply given by the normalization of the exact wave function $S(N) = \langle\tilde{\Psi}|\tilde{\Psi}\rangle^{-1/2}$ and can be cast in the convenient form

$$\begin{aligned}S(N) &= (1 + \langle\Delta\Psi|\Delta\Psi\rangle)^{-1/2}, \\ |\Delta\Psi\rangle &= \sum_{n=1}|\tilde{\Psi}^{(n)}\rangle, \quad (11)\end{aligned}$$

where $|\Delta\Psi\rangle = |\Psi\rangle - |N\rangle$ is the correction to the mean-field wave function.

Using the leading term of perturbation theory for the wave function provides the leading term of the overlap:

$$\begin{aligned}S(N) &= (1+\Lambda^2\alpha^2)^{-1/2}, \\ \alpha^2 &= \frac{\langle\Psi^{(1)}|\Psi^{(1)}\rangle}{\Lambda^2} = \frac{N}{2(N-1)}\sum_{i,j}\frac{|V_{ij00}|^2}{(2\mu_0-\mu_i-\mu_j)^2}. \quad (12)\end{aligned}$$

Here and in the following, unless explicitly indicated, all one-particle indexes refer to orbitals outside the condensed manifold, e.g., $i = 1,2,\ldots$. Note that there is a misprint in the respective equation in [12]. Again, also the overlap $S(N)$ is well behaved as a function of N and for large N coincides with the result in [12]. Since all the integrals V_{ijkl} and the orbital energies μ_s depend on Λ, but not on N, the overlap tends fast to its large-N value as is also the case for other many-body quantities beyond the mean field. It has been demonstrated in [12] that the overlap in Eq. (11) can be very small and even vanish.

3. *The depletion of the condensate*

Usually, the depletion of a condensate is defined as the fraction of the system which is not condensed. In [22] it has been shown that under certain conditions the system is 100% condensed in the limit of infinite particles keeping the interaction strength Λ fixed. As found in [12] and demonstrated in the next section more generally, the depletion is essentially a constant; i.e., one should rather define and compute it in absolute terms and not as a fractional term. Each of the particles outside the condensed manifold interacts with all the particles of the condensate and this gives rise to the sometimes enormous impact on the full wave function. Although the depletion can be related to any exact state of the system, we confine ourself for transparency to the ground state.

Defining the depletion $D(\Lambda)$ as the number of particles outside the condensed manifold, the number of condensed bosons is $\langle\Psi|b_0^\dagger b_0|\Psi\rangle$. Since the particle-number operator can be written as $\hat{N} = \sum_{q=0} b_q^\dagger b_q$, the depletion can be expressed as

$$\begin{aligned}D(\Lambda) &= N - \langle\Psi|b_0^\dagger b_0|\Psi\rangle \\ &= \langle\Psi|\sum_{i=1} b_i^\dagger b_i|\Psi\rangle. \quad (13)\end{aligned}$$

To evaluate the depletion to the leading order of perturbation theory, we just have to notice that applying the depletion operator $\hat{D} = \sum_{i=1} b_i^\dagger b_i$ to the mean-field state $|N\rangle$ vanishes. One is thus left with $D = \langle\tilde{\Psi}^{(1)}|\hat{D}|\tilde{\Psi}^{(1)}\rangle$ which is easily evaluated explicitly to give

$$D(\Lambda) = 2\langle\tilde{\Psi}^{(1)}|\tilde{\Psi}^{(1)}\rangle = 2\Lambda^2\alpha^2 \geqslant 0, \quad (14)$$

where α^2 can be found in Eq. (12). It is seen that to the leading order of perturbation theory, both the overlap between the exact and mean-field wave functions and the depletion are determined by the same quantity $\Lambda^2\alpha^2$. Following [12], α^2 generally reflects the space available for the bosons. The more space is available the smaller the overlap S and the larger the depletion D are. We also stress that the depletion does not depend on the boson number once this number is large.

4. The boson correlation energy

The energy increment beyond the mean-field energy is the boson correlation energy, or briefly, correlation energy:

$$E_c = E_{\mathrm{MF}} - E_{\mathrm{exact}}.$$

The definition is such that the correlation energy is a positive quantity. The explicit expression for the mean-field energy can be found below Eq. (9).

To the leading order in the interaction strength, the correlation energy can simply be obtained from Eq. (9) using the first-order correction to the wave function $\tilde{\Psi}^{(1)}$ which is provided explicitly in Eq. (10). The result takes on the simple appearance

$$-E_c = E^{(2)} = \frac{\Lambda^2}{2}\frac{N}{N-1}\sum_{i,j}\frac{|V_{ij00}|^2}{2\mu_0-\mu_i-\mu_j} \leqslant 0. \quad (15)$$

Again, we see that the dependence on the boson number is only via the fraction $N/(N-1)$, i.e., the correlation energy is, for a fixed interaction strength, essentially a constant. This *strongly* contrasts the situation for fermions where the correlation energy is an extensive quantity for large N, i.e., grows with the number of fermions for large N [41].

5. The reduced one-body density matrix

The reduced one-body density matrix, which we shall briefly call the density matrix, can be written as [3,42]

$$\rho(\mathbf{r},\mathbf{r}') = \langle\Psi|\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r}')|\Psi\rangle,$$

where $\hat{\Psi}(\mathbf{r}) = \sum_{i=0}\varphi_i(\mathbf{r})b_i$ is the field operator. Inserting into the above equation, one readily finds that the density matrix is composed of three terms of different behavior

$$\rho(\mathbf{r},\mathbf{r}') = \varphi_0(\mathbf{r})^*\varphi_0(\mathbf{r}')\rho_{00} + \Bigg[\sum_i \varphi_0(\mathbf{r})^*\varphi_i(\mathbf{r}')\rho_{0i} + \mathrm{c.c.}(\mathbf{r}'\leftrightarrow\mathbf{r})\Bigg] + \sum_{i,j}\varphi_i(\mathbf{r})^*\varphi_j(\mathbf{r}')\rho_{ij}, \quad (16)$$

where

$$\rho_{ij} = \langle\Psi|b_i^\dagger b_j|\Psi\rangle$$

are the matrix elements of the density matrix. Following Bogoliubov [3,27], for large N the first term on the right-hand side of the above equation should scale as N, the second as $\sqrt{N}$, and the third term, which describes the particles outside the condensed part of the system, as a constant. We shall see below what happens if the mean field is used as the unperturbed operator.

In the following we compute the leading term in perturbation theory of all the matrix elements ρ_{ij}. It is straightforward to show that there is no contribution of first order in Λ because of the mean-field used. A typical first-order term is an element of the form $\langle N|b_i^\dagger b_j|\tilde{\Psi}^{(1)}\rangle$ which vanishes either because of the intermediate normalization employed or because $|\tilde{\Psi}^{(1)}\rangle$ does not contain singly excited configurations [see Eq. (10)].

Up to second order we already know the answer for ρ_{00} of the condensed manifold (see Sec. II C 3):

$$\rho_{00} = N - D,$$

where D is the depletion. Similarly, one finds that $\langle\tilde{\Psi}^{(1)}|b_i^\dagger b_j|\tilde{\Psi}^{(1)}\rangle$ vanishes unless both i and j are $\geqslant 1$ and also that all $\langle\tilde{\Psi}^{(2)}|b_i^\dagger b_j|N\rangle$ vanish except for $j=0$. Consequently, the leading terms of the remaining matrix elements are

$$\rho_{ij} = \langle\tilde{\Psi}^{(1)}|b_i^\dagger b_j|\tilde{\Psi}^{(1)}\rangle,$$

for i and $j \geqslant 1$, and

$$\rho_{i0} = \rho_{0i}^* = \langle\tilde{\Psi}^{(2)}|b_i^\dagger b_0|N\rangle,$$

for $i \geqslant 1$.

We begin with ρ_{ij}. As $|\tilde{\Psi}^{(1)}\rangle$ is explicitly known, see Eq. (10), the evaluation is straightforward. By applying the destruction operator b_j to the first-order correction of the state one obtains

$$b_j|\tilde{\Psi}^{(1)}\rangle = \Lambda\sqrt{\frac{N}{(N-1)}}\sum_k\frac{V_{jk00}}{2\mu_0-\mu_k-\mu_j}|N-2,1_k\rangle,$$

and ρ_{ij} is determined by taking the scalar product with the same quantity, but where j is replaced by i. To the leading order in Λ one thus finds for i and $j \geqslant 1$

$$\rho_{ij} = \Lambda^2\frac{N}{(N-1)}\sum_k\frac{V_{ik00}^*V_{jk00}}{(2\mu_0-\mu_k-\mu_i)(2\mu_0-\mu_k-\mu_j)}. \quad (17)$$

For large N these matrix elements of the density matrix are constants as expected from Bogoliubov theory.

We now turn to the last group of elements, ρ_{0i}, which are of particular importance as they connect the condensed manifold to the uncondensed part of the system. There is no need to compute the cumbersome second-order correction $|\tilde{\Psi}^{(2)}\rangle$ explicitly in order to determine the leading term in the perturbation expansion of ρ_{0i}. Because $\langle N|b_0^\dagger b_i = \sqrt{N}\langle N-1,1_i|$, it suffices to operate with $\lambda_0 W$ on this singly excited configuration and then take the scalar product with $|\tilde{\Psi}^{(1)}\rangle$; see Eq. (8). As can be seen in Eq. (10), the latter quantity contains only doubly excited configurations and, therefore, one needs to compute only such configurations when operating with $\lambda_0 W$ on $\langle N-1,1_i|$. The calculation is somewhat lengthy but straightforward, and we refrain from showing all the steps and just provide the final result for the leading order in Λ:

$$\rho_{0i} = \frac{\Lambda^2}{\mu_0-\mu_i}\frac{N}{(N-1)}A,$$
$$A = \sum_{k,l}\frac{V_{kli0}^*V_{kl00}}{2\mu_0-\mu_k-\mu_l} - \sum_k\frac{V_{k000}^*V_{ki00}}{2\mu_0-\mu_k-\mu_i}. \quad (18)$$

Following Bogoliubov theory, ρ_{0i} is expected to scale as $\sqrt{N}$ for large N. However, due to the choice of the unperturbed Hamiltonian, this quantity scales like a constant N^0.

Let us briefly discuss some consequences. Diagonalizing the density matrix is equivalent to diagonalizing the matrix $\{\rho_{ij}\}$, $i,j \geqslant 0$, defining new orbitals ϕ named *natural orbitals* in which $\rho(\mathbf{r},\mathbf{r}')$ takes on the appearance

$$\rho(\mathbf{r},\mathbf{r}') = \sum_{i=0} n_i \phi_i(\mathbf{r})^* \phi_i(\mathbf{r}'),$$

where the n_i are the corresponding *natural occupations* [42–44]. We remind the reader that the one-particle density $\rho(\mathbf{r}) = \rho(\mathbf{r},\mathbf{r})$ has a particularly appealing appearance in this representation as a sum of weighted orbital densities: $\rho(\mathbf{r}) = \sum_{i=0} n_i |\phi_i(\mathbf{r})|^2$. For very large N Bogoliubov scaling would tell us that in the matrix $\{\rho_{ij}\}$, the element ρ_{00} will decouple from ρ_{ij}, $i,j \geqslant 1$ because the former scales as N, the latter as constants, and the elements ρ_{0j}, $j \geqslant 1$, coupling these two sets, scale as $\sqrt{N}$. In the limit $N \to \infty$ it becomes clear that the natural orbital ϕ_0 will become identical to the mean-field orbital φ_0 and its occupation will be $n_0 = N - D$. This connects the above definition of the depletion with the traditional measure based on the natural occupations. As we have seen above, the coupling elements also scale as a constant, and, consequently, the mean-field orbital will become essentially identical to the respective natural orbital already at much smaller N. In the examples studied in [12] this is already the case for $\sim 10^3$–10^4 bosons.

III. MANY-BODY THEORY FOR TRAPPED BOSONS IN THE INFINITE-PARTICLE LIMIT

A. The reduction of the Hamiltonian

In the infinite-particle limit one can simplify the full Hamiltonian (5) in the spirit of Bogoliubov by expanding it in N and retaining the leading orders. Being interested in bosons in a trap potential, we study the limit $N \to \infty$ keeping the interaction strength Λ fixed [17,29,30] and not the thermodynamic limit investigated by Bogoliubov for homogeneous systems [27]. The situation is discussed in some detail in the introduction. It will be shown below that using the mean field as the unperturbed Hamiltonian as derived in the preceding section automatically leads to a particle-conserving theory for large N and for any boson-boson interaction potential.

As the full Hamiltonian commutes with the particle-number operator $\hat{N}$, we can add to it, without loss of generality, the quantity $\mu_0(N - \hat{N})$, which vanishes when applied to a state of N bosons. To proceed, we rewrite the Hamiltonian (5) as

$$H = \mu_0 N + \sum_i (\mu_i - \mu_0) b_i^\dagger b_i + \sum_{n=1}^{6} \lambda_0 W_n, \tag{19a}$$

where we collect in each of the terms $\lambda_0 W_n$ all the parts of the boson-boson interaction $\lambda_0 W$ with a given number of operators $b_0^\dagger$ and b_0 related to the condensed part of the system. For brevity we call them 0-operators. Since $\Lambda = \lambda_0(N-1)$, it is also counted as if it would contain a product $b_0^\dagger b_0$. Introducing the condensate-number operator $\hat{n}_0 = b_0^\dagger b_0$, one finds for the term which contains four 0-operators

$$\lambda_0 W_1 = \hat{n}_0 \left[\frac{\lambda_0}{2}(\hat{n}_0 - 1) - \Lambda \right] V_{0000}, \tag{19b}$$

and for the term containing three 0-operators

$$\lambda_0 W_2 = b_0 [\lambda_0(\hat{n}_0 - 1) - \Lambda] \sum_i V_{i000} b_i^\dagger + \text{H.c.} \tag{19c}$$

There are three contributions which contain two 0-operators, but because we would like each of the $\lambda_0 W_n$ terms to be Hermitian, we combine two of them together and obtain

$$\lambda_0 W_3 = \sum_{i,j} [\lambda_0 \hat{n}_0 (V_{i0j0} + V_{i00j}) - \Lambda V_{i0j0}] b_i^\dagger b_j, \tag{19d}$$

$$\lambda_0 W_4 = (b_0)^2 \left[\frac{\lambda_0}{2} \sum_{i,j} V_{ij00} b_i^\dagger b_j^\dagger \right] + \text{H.c.} \tag{19e}$$

Similarly, there are two contributions with a single 0-operator which are Hermitian conjugate of each other and one contribution without any 0-operator:

$$\lambda_0 W_5 = b_0 \left[\lambda_0 \sum_{i,j,k} V_{ijk0} b_i^\dagger b_j^\dagger b_k \right] + \text{H.c.}, \tag{19f}$$

$$\lambda_0 W_6 = \frac{\lambda_0}{2} \sum_{i,j,k,l} V_{ijkl} b_i^\dagger b_j^\dagger b_l b_k. \tag{19g}$$

We remind the reader that unless otherwise indicated all indexes are $\geqslant 1$.

Now, we are in the position to consider a condensate with very large N and replace in the Hamiltonian (19a) the operators b_0 and $b_0^\dagger$ by $\sqrt{N}$, and, of course, $\hat{n}_0$ by N. The first term becomes just a number $\lambda_0 W_1 = -\frac{\Lambda N}{2} V_{0000}$. The second term of the boson-boson interaction vanishes identically because of the choice of mean field as the unperturbed Hamiltonian: $\lambda_0 W_2 = 0$. Because of the identity $\Lambda = \lambda_0(N-1)$, the fifth term $\lambda_0 W_5$ gets a prefactor of $\frac{\Lambda}{\sqrt{N}}$ and the sixth term $\lambda_0 W_6$ of $\frac{\Lambda}{N}$ and both terms vanish too in the limit $N \to \infty$. We are left with the third and fourth terms as operators only. They now take on the simple appearance

$$\lambda_0 W_3 = \Lambda \sum_{i,j} V_{i00j} b_i^\dagger b_j, \tag{20a}$$

$$\lambda_0 W_4 = \frac{\Lambda}{2} \sum_{i,j} V_{ij00} b_i^\dagger b_j^\dagger + \frac{\Lambda}{2} \sum_{i,j} V_{00ij} b_i b_j. \tag{20b}$$

The rather complex Hamiltonian (19a) has thus been reduced in the infinite-particle limit to the much less complex Hamiltonian

$$\begin{aligned} H = &\left[\mu_0 N - \frac{\Lambda N}{2} V_{0000} \right] + \sum_i (\mu_i - \mu_0) b_i^\dagger b_i \\ &+ \Lambda \sum_{i,j} V_{i00j} b_i^\dagger b_j + \frac{\Lambda}{2} \sum_{i,j} V_{ij00} b_i^\dagger b_j^\dagger \\ &+ \frac{\Lambda}{2} \sum_{i,j} V_{00ij} b_i b_j. \end{aligned} \tag{21}$$

Above, the number in brackets is nothing but the mean-field energy E_{MF} discussed in Sec. II B. The next term is the

unperturbed Hamiltonian operating in the boson space outside the condensed manifold, and the remaining terms describe the interaction of the particles outside of this manifold. We mention that the reduction of the Hamiltonian has been possible strictly because the depletion and correlation energy scale as N^0. Indeed, apart from the trivial number $E_{\rm MF}$, the reduced Hamiltonian does not exhibit terms depending on N. The only memory of the condensate manifold is found in the direct interaction matrix elements V_{ij00} and in the exchange matrix elements V_{i00j} which describe the interaction of the "depleted bosons" with the "infinite sea" of the condensate manifold. This interaction with the condensate manifold mediates the interaction between the depleted bosons themselves. We stress again that in spite of the vanishing depleted fraction $\frac{D}{N}$ as $N \to \infty$, this interaction leads to a generally very complex wave function of the condensate.

1. Conservation of the number of particles

As already discussed in the introduction, the theory of Bogoliubov [3,27] is for the thermodynamic limit of homogeneous systems and Fetter [30] has extended the theory to apply for spatially inhomogeneous condensates. These theories are not number conserving and have been extended to become a number-conserving Bogoliubov theory by Girardeau [28] and by Gardiner [29] who has also extended the theory of Fetter for spatially inhomogeneous condensates to a particle-conserving one.

Following Gardiner, it is not the bare operator b_0 which gives $\sqrt{N}$ when acting on a state with a total number of bosons N, but rather an operator A. For large N the relationship between these two operators can be cast as

$$b_0 = A\left[1 - \frac{\sum_{i=1} b_i^\dagger b_i}{2N}\right]. \tag{22}$$

Correspondingly, the action of $\hat{n}_0$ has to be replaced by that of $\hat{N} - \sum_{i=1} b_i^\dagger b_i$ or, equivalently, by $N - \hat{D}$, where $\hat{D}$ is the depletion operator discussed in Secs. II C 3 and II C 5. By applying these relationships to the Hamiltonian, Gardiner has obtained the corrections which make the Bogoliubov theory particle-number conserving.

We now apply these relationships to the full Hamiltonian (19a) to find out whether corrections to the reduced Hamiltonian (21) are necessary. It is only necessary to investigate the term $\lambda_0 W_1$ which contains the most possible number of 0-operators and is thus, according to Gardiner, prone to corrections. $\lambda_0 W_1$ is the difference of the two terms $\frac{\lambda_0}{2}\{[(\hat{n}_0)^2 - \hat{n}_0]\}V_{0000}$ and $\Lambda \hat{n}_0 V_{0000}$, where the second stems from the mean-field interaction. Inserting the expression above of Gardiner into the first term gives $\frac{\lambda_0}{2}[N(N-1) - 2N\hat{D}]V_{0000}$ and thus $\frac{\Lambda}{2}[N - 2\hat{D}]V_{0000}$. The second term gives immediately $\Lambda[N - \hat{D}]V_{0000}$. Clearly, the difference of the two terms is just $-\frac{N\Lambda}{2}V_{0000}$ as found above. In other words, the reduction of $\lambda_0 W_1$ is invariant to applying Gardiner's correction and clearly this is due to the choice of the unperturbed Hamiltonian.

Therefore, the reduction of the full Hamiltonian as performed in the previous subsection is invariant to applying Gardiner's correction. The reason for the invariance of the remaining terms is due to the fact that a factor N is needed to make λ_0, appearing in all the expressions, become Λ. Therefore, a correction as in Eq. (22) does not suffice to introduce an additional term into the Hamiltonian which does not vanish for $N \to \infty$.

2. Mapping the reduced Hamiltonian on a system of coupled phonons

As it stands, the reduced Hamiltonian (21) describes a system of coupled oscillators. We would like to recast this Hamiltonian by mapping it on a Hamiltonian describing phonons or molecular vibrations. In this case, the interaction potential is expanded in the vibrational coordinates and momentum coupling due to the kinetic energy is also possible; see for instance [45]. As usual, the vibrational coordinate of the jth vibrational mode describing the distortion from equilibrium is $x_j = \frac{1}{\sqrt{2}}(b_j + b_j^\dagger)$ and the momentum of this mode is $p_j = \frac{i}{\sqrt{2}}(b_j - b_j^\dagger)$. Expressing the expansion of the reduced Hamiltonian in these combinations of the destruction and creation operators for bosons sheds additional light on its physics, and also serves to solve the underlying problem, i.e., diagonalize the Hamiltonian, using methods applied for molecular vibrations.

The general Hamiltonian describing molecular vibrations and expanded up to second order in the coordinates and momenta takes on the following appearance [45]:

$$H = C_E + \sum_i \omega_i (b_i^\dagger b_i + 1/2) + \sum_{i,j} \gamma_{ij}(b_i + b_i^\dagger)(b_j + b_j^\dagger) + \sum_{i,j} \tau_{ij}(b_i - b_i^\dagger)(b_j - b_j^\dagger), \tag{23}$$

where C_E is a constant and symmetry-breaking linear terms have been excluded.

Multiplying the operators appearing in this equation and making use of the usual commutation relations of boson operators $[b_i, b_j^\dagger] = \delta_{ij}$ and $[b_i, b_j] = 0$ leads to a form as in Eq. (21). By equating the two expressions, one finds

$$\begin{aligned} \gamma_{ij} &= \frac{\Lambda}{4}\left[V_{ij00} + V_{i00j}\right], \quad \tau_{ij} = \frac{\Lambda}{4}\left[V_{ij00} - V_{i00j}\right], \\ \omega_i &= (\mu_i - \mu_0), \\ C_E &= E_{\rm MF} - \sum_i \frac{(\mu_i - \mu_0)}{2} - \sum_i \frac{\Lambda}{2} V_{i00j}, \end{aligned} \tag{24}$$

where $E_{\rm MF}$ is as before the mean-field energy. To derive the above relations, we have assumed that V_{ij00} is real which is only a minor restriction; the orbitals do not have to be real to fulfill this condition. The coupling of the modes through the interaction potential is described by the coupling constants γ_{ij} while the coupling through the kinetic energy operator is by τ_{ij}. Interestingly, if the orbitals used are real, $V_{ij00} = V_{i00j}$ and the latter couplings vanish. As the orbitals are the eigenfunctions of the Fock operator (3), the problem at hand tells us whether the orbitals are real or complex. For instance, for interacting bosons on a ring the orbitals are also eigenfunctions of the angular momentum operator and hence complex.

B. Diagonalization of the reduced Hamiltonian

To proceed we rewrite the Hamiltonian in matrix notation. For that purpose we follow [45] and collect the destruction and creation operators in a single column vector $\mathbf{B}$, and introduce the 2×2 supermatrices $\mathbf{\Gamma}$, $\mathbf{T}$, and $\mathbf{\Omega}$ which have as elements the matrices of the coupling constants $\boldsymbol{\gamma} = \{\gamma_{ij}\}$, $\boldsymbol{\tau} = \{\tau_{ij}\}$ and the diagonal matrix $\boldsymbol{\omega}$ of the frequencies ω_i, respectively. More precisely,

$$\mathbf{B} = \begin{pmatrix} b_1 \\ b_2 \\ . \\ . \\ . \\ b_1^\dagger \\ b_2^\dagger \\ . \\ . \\ . \end{pmatrix}, \qquad \mathbf{\Gamma} = \begin{pmatrix} \boldsymbol{\gamma} & \boldsymbol{\gamma} \\ \boldsymbol{\gamma} & \boldsymbol{\gamma} \end{pmatrix},$$

$$\mathbf{T} = \begin{pmatrix} -\boldsymbol{\tau} & \boldsymbol{\tau} \\ \boldsymbol{\tau} & -\boldsymbol{\tau} \end{pmatrix}, \qquad \mathbf{\Omega} = \begin{pmatrix} \boldsymbol{\omega} & 0 \\ 0 & \boldsymbol{\omega} \end{pmatrix}. \tag{25}$$

With this notation the phonon Hamiltonian in Eq. (23) can be cast into the following compact form:

$$H = C_E + \tfrac{1}{2}\mathbf{B}^\dagger \mathbf{\Omega} \mathbf{B} + \mathbf{B}^\dagger(\mathbf{\Gamma} + \mathbf{T})\mathbf{B}, \tag{26}$$

which is amenable to diagonalization.

The diagonalization procedure

By defining new boson operators c_i which fulfill the usual commutation relations for bosons, one can bring the phonon Hamiltonian (26) into diagonal form:

$$H = C_E + \tfrac{1}{2}\mathbf{C}^\dagger \bar{\mathbf{\Omega}} \mathbf{C}, \tag{27}$$

where the vector $\mathbf{C}$ is defined in analogy to $\mathbf{B}$ and $\bar{\mathbf{\Omega}}$ is the same as $\mathbf{\Omega}$ in Eq. (25), but with the new frequencies $\bar{\omega}_i$ on the diagonal. The diagonalization procedure is described in [45] and we only give here the equations needed.

Because of the structure of the vectors $\mathbf{B}$ and $\mathbf{C}$, we have

$$\mathbf{C} = \mathbf{\Xi}\mathbf{B}, \qquad \mathbf{\Xi} = \begin{pmatrix} \mathbf{\Xi}_1 & \mathbf{\Xi}_2 \\ \mathbf{\Xi}_2 & \mathbf{\Xi}_1 \end{pmatrix}. \tag{28}$$

Due to commutation relations of the c_i, one finds that the inverse of the transformation matrix $\mathbf{\Xi}$ takes on the following appearance:

$$\mathbf{\Xi}^{-1} = \begin{pmatrix} \mathbf{\Xi}_1^\dagger & -\mathbf{\Xi}_2^\dagger \\ -\mathbf{\Xi}_2^\dagger & \mathbf{\Xi}_1^\dagger \end{pmatrix}. \tag{29}$$

The transformation matrix $\mathbf{\Xi}$, of course, also determines the transformation matrix $\mathbf{J}$ which transforms the old vibrational coordinates $x_i = \frac{1}{\sqrt{2}}(b_i + b_i^\dagger)$ into the new ones $\bar{x}_i = \frac{1}{\sqrt{2}}(c_i + c_i^\dagger)$. It reads

$$\mathbf{J} = \mathbf{\Xi_1} + \mathbf{\Xi_2}, \qquad \mathbf{J}^{-\mathbf{1}^\dagger} = \mathbf{\Xi_1} - \mathbf{\Xi_2}. \tag{30}$$

Imposing the frequency matrix $\bar{\mathbf{\Omega}}$ to be diagonal leads to an explicit expression for the transformation matrix $\mathbf{J}$:

$$\mathbf{J} = \bar{\boldsymbol{\omega}}^{\frac{1}{2}} \mathbf{Z} (\boldsymbol{\omega} - 4\boldsymbol{\tau})^{-\frac{1}{2}}, \tag{31}$$

where $\mathbf{Z}$ is an unitary matrix determined as the eigenvector matrix of the following eigenvalue problem

$$(\boldsymbol{\omega} - 4\boldsymbol{\tau})^{\frac{1}{2}} (\boldsymbol{\omega} + 4\boldsymbol{\gamma}) (\boldsymbol{\omega} - 4\boldsymbol{\tau})^{\frac{1}{2}} \mathbf{Z}^\dagger = \mathbf{Z}^\dagger \bar{\boldsymbol{\omega}}^2. \tag{32}$$

It is seen that the new frequencies, i.e., the frequencies of the diagonalized Hamiltonian, are the eigenvalues in the above eigenvalue equation. Since the supermatrix $\mathbf{\Xi}$ which transforms the boson operators b_i to the c_i diagonalizing the phonon Hamiltonian is determined by $\mathbf{J}$, see Eq. (30), solving the above eigenvalue equation completes the task of diagonalizing this Hamiltonian.

C. Properties

In Sec. II C we discussed a number of properties of physical relevance and derived for each of them the leading term in the perturbative expansion in the interaction strength Λ. In the present subsection we derive explicit expressions for the same properties, but now in the infinite-particle limit.

For compactness the discussion below is for the ground state of the system, but we mention that the approach can also be used for excited states. Because the reconstruction of the wave function is different from that for the other properties, we first discuss these properties and then the wave function in the proceeding section.

1. The overlap of the mean-field and exact wave functions

In contrast to the general situation discussed in section II where the mean-field ground state is $|N\rangle$, let us name the mean-field ground state in the infinite-particle limit by $|0\rangle$. Indeed, this is the ground state of the unperturbed reduced Hamiltonian $\sum_i (\mu_i - \mu_0) b_i^\dagger b_i$ in Eq. (21). Similarly, we denote by $|\bar{0}\rangle$ the ground-state solution of the reduced Hamiltonian (21) or equivalently, of the phonon Hamiltonian (27).

The overlap S of the mean-field and exact wave function in the limit $N \to \infty$ is thus given by $\langle 0|\bar{0}\rangle$ and can be explicitly expressed by $\mathbf{\Xi}_1$ alone [45]:

$$S = [\det(\mathbf{\Xi}_1)]^{-\frac{1}{2}}, \tag{33}$$

where $\det(\mathbf{\Xi}_1)$ is the determinant of the matrix $\mathbf{\Xi}_1$.

2. The depletion of the condensate

The depletion D in the ground state is the expectation value of the depletion operator $\langle\bar{0}| \sum_{i=1} b_i^\dagger b_i |\bar{0}\rangle$. We can first use the matrix notation in Eq. (25) to express the depletion operator (up to a constant which will cancel out later) simply as $\frac{1}{2}\mathbf{B}^\dagger\mathbf{B}$, and subsequently rewrite this quantity employing the transformation in Eq. (28) to obtain $\frac{1}{2}\mathbf{C}^\dagger \mathbf{\Xi}^{-1^\dagger} \mathbf{\Xi}^{-1} \mathbf{C}$. The

appearing inverse matrices can be expressed via Eq. (29). Now, when applied to the exact ground state of the phonon Hamiltonian we can make use of the fact that in this state there are no phonons occupied and thus $c_i|\bar{0}\rangle = 0$, and consequently we have to collect only the contributions with $\langle\bar{0}|c_i \ldots c_i^\dagger|\bar{0}\rangle$. This leads to

$$D = \tfrac{1}{2}\mathrm{Tr}[\boldsymbol{\Xi}_1\boldsymbol{\Xi}_1^\dagger + \boldsymbol{\Xi}_2\boldsymbol{\Xi}_2^\dagger - 1],$$

where Tr[**X**] is the trace of the matrix **X**.

This expression can be further simplified. Because of the identity $\boldsymbol{\Xi}^{-1}\boldsymbol{\Xi} = 1$ and the relation (29), one readily finds the final result for the depletion:

$$D = \mathrm{Tr}[\boldsymbol{\Xi}_2\boldsymbol{\Xi}_2^\dagger]. \tag{34}$$

The physical meaning of this equation becomes more evident when realizing that $\boldsymbol{\Xi}_2$ shows the contribution of the creation operators $b_i^\dagger$ of mean-field phonons to the annihilation operators c_i of the exact phonons; see Eqs. (25) and (28).

3. The boson correlation energy

The ground-state energy of the phonon Hamiltonian is, of course, given by the sum of the zero-point energies of the oscillators. For $\frac{1}{2}\mathbf{C}^\dagger\bar{\boldsymbol{\Omega}}\mathbf{C}$ this energy is simply $\frac{1}{2}\sum_i \bar{\omega}_i$. With the explicit expression for C_E in Eq. (24), the correlation energy takes on the following appearance:

$$E_c = \sum_i \frac{\Lambda}{2} V_{i00j} + \frac{1}{2}\sum_i(\omega_i - \bar{\omega}_i). \tag{35}$$

To better understand the first term in the correlation energy, we expand the eigenvalue equation (32) for the vibrational frequencies $\bar{\omega}_i$ for small values of the interaction strength Λ. The leading term in Λ is linear and is obtained by considering only the diagonal part. For $1 \gg \Lambda$, a diagonal element of the matrix to be diagonalized in Eq. (32) becomes

$$\begin{aligned}\bar{\omega}_i^2 &= (\omega_i - 4\tau_{ii})^{\frac{1}{2}}(\omega_i + 4\gamma_{ii})(\omega_i - 4\tau_{ii})^{\frac{1}{2}} \\ &= {\omega_i}^2[1 + 4(\gamma_{ii} - \tau_{ii})/\omega_i] + \cdots .\end{aligned}$$

Taking the square root of $\bar{\omega}_i$ above gives

$$\bar{\omega}_i = \omega_i + 2(\gamma_{ii} - \tau_{ii}) + \cdots ,$$

which, when inserted into the second term on the right-hand side of Eq. (35), exactly compensates the first term. What remains in the expansion of the correlation energy are terms of the order Λ^2 and higher.

4. The reduced one-body density matrix

The general aspects of the elements ρ_{ij} of the density matrix $\boldsymbol{\rho}$ have been discussed in Sec. II C 5. To compute them in the infinite-particle limit, we start from $\rho_{ij} = \langle\bar{0}|b_i^\dagger b_j|\bar{0}\rangle$ and notice that $\langle\bar{0}|\mathbf{B}\mathbf{B}^\dagger|\bar{0}\rangle$ defines a 2×2 supermatrix and the density matrix is just the lower-right element of this supermatrix. Using Eqs. (28) and (29) one can express the lower-right element of $\mathbf{B}\mathbf{B}^\dagger$ as a linear combination of matrices with elements $c_i^\dagger c_j, c_i c_j, c_i^\dagger c_j^\dagger$, and $c_i c_j^\dagger$. When taking the expectation values of these matrices with the ground state $|\bar{0}\rangle$ all terms except the expectation value of the latter vanish. The result simply reads

$$\boldsymbol{\rho} = \boldsymbol{\Xi}_2^\dagger\boldsymbol{\Xi}_2. \tag{36a}$$

While $\langle\bar{0}|c_i c_j|\bar{0}\rangle$ vanishes identically, it is interesting to note that $\langle\bar{0}|b_i b_j|\bar{0}\rangle$ does not. The latter is a measure for the influence of the non-particle-conserving term $\lambda_0 W_4$ (20b) in the Hamiltonian (19a) and hence for the complexity of the exact state. The matrix $\tilde{\boldsymbol{\rho}}$ with elements $\tilde{\rho}_{ij} = \langle\bar{0}|b_i b_j|\bar{0}\rangle$ is the upper-right element of the supermatrix $\langle\bar{0}|\mathbf{B}\mathbf{B}^\dagger|\bar{0}\rangle$. Similarly to the above, one can compute this matrix and obtain

$$\tilde{\boldsymbol{\rho}} = -\boldsymbol{\Xi}_1^\dagger\boldsymbol{\Xi}_2. \tag{36b}$$

D. Reconstruction of the wave function in the infinite-particle limit

We show here that, in principle, one can also reconstruct the full particle-conserving wave function for large N, i.e., of the full Hamiltonian and not just of the phonon Hamiltonian derived in Secs. III A and III B. The wave function of the phonon Hamiltonian is, of course, not particle-number conserving as it describes the dynamics of the bosons outside the condensed manifold. As far as we know, the determination of the full wave function out of the wave function in the phonon approximation has not been discussed before.

First, let us write the exact eigenstates of the reduced Hamiltonian (21) or, equivalently, of the phonon Hamiltonian (26) explicitly as

$$|\bar{n}_1,\bar{n}_2,\bar{n}_3\ldots\rangle = \frac{(c_1^\dagger)^{\bar{n}_1}(c_2^\dagger)^{\bar{n}_2}(c_3^\dagger)^{\bar{n}_3}\cdots}{\sqrt{\bar{n}_1!\bar{n}_2!\bar{n}_3!\cdots}}|\bar{0}\rangle. \tag{37a}$$

This equation requires some discussion. In Sec. II the full Hamiltonian describing interacting particles has been discussed whose eigenstates are particle-number conserving and hence the eigenstates of the unperturbed Hamiltonian there were the particle-number-conserving Fock states given in Eq. (6). In contrast, the eigenstates of the phonon Hamiltonian are not particle conserving as common for phonon systems. In other words, the sum of the occupation numbers $\sum_i \bar{n}_i$ can take on any integer, 0,1,2, ..., value. In contrast to Eq. (6), where the creation operators act on the vacuum state $|\mathrm{vac}\rangle$ of no particles, the $c_i^\dagger$ operators which diagonalize the phonon Hamiltonian, see Eq. (27), act in the above eigenstate on $|\bar{0}\rangle$ which is the exact ground state (zero c-phonons) of this Hamiltonian.

With this important difference in mind, we may now write down the phonon states of the unperturbed phonon operator $\frac{1}{2}\mathbf{B}^\dagger\Omega\mathbf{B}$ in Eq. (26) using the original creation operators $b_i^\dagger$, $i \geqslant 1$, for particles outside the condensed manifold which now play the role of phonons as well:

$$|n_1,n_2,n_3\ldots\rangle = \frac{(b_1^\dagger)^{n_1}(b_2^\dagger)^{n_2}(b_3^\dagger)^{n_3}\cdots}{\sqrt{n_1!n_2!n_3!\cdots}}|0\rangle. \tag{37b}$$

Again, as above in Eq. (37a), the sum of the occupations numbers $\sum_i n_i$ can be an arbitrary integer. The state $|0\rangle$ on which the $b_i^\dagger$ operate is the ground state (zero b-phonons) of $\frac{1}{2}\mathbf{B}^\dagger\Omega\mathbf{B}$. The two states $|0\rangle$ and $|\bar{0}\rangle$ differ from each other. Their overlap has been given in Eq. (33).

Any eigenstate $|\bar{n}_1,\bar{n}_2,\bar{n}_3,\ldots\rangle$ of the phonon Hamiltonian can be expanded in the eigenstates $|n_1,n_2,n_3,\ldots\rangle$. For brevity, we discuss only that of the ground state $|\bar{0}\rangle$ as the expansion of other states is similar. The expansion reads

$$|\bar{0}\rangle = \sum_{n_1=0,n_2=0,\ldots} |n_1,n_2,n_3,\ldots\rangle C_{n_1,n_2,\ldots},$$
$$C_{n_1,n_2,\ldots} = \langle n_1,n_2,n_3,\ldots|\bar{0}\rangle.$$

To proceed, we note that the eigenstate of the phonon Hamiltonian is now expressed in the first line of the above equation via operators $b_i^\dagger$. These operators are the operators which appear in the full Hamiltonian (5). These operators thus relate also to particles and we may augment each Fock state $|n_1,n_2,n_3,\ldots\rangle$ uniquely to include also the particles in the condensate manifold, such that the total number of particles is equal to N. Let the total number of phonons in an arbitrary Fock state $|n_1,n_2,n_3,\ldots\rangle$ be $\mathcal{P}_{n_1,n_2,\ldots} = \sum_i n_i$; then the unique assignment

$$|n_1,n_2,n_3,\ldots\rangle \Longrightarrow |N-\mathcal{P}_{n_1,n_2,\ldots},n_1,n_2,n_3,\ldots\rangle \tag{38a}$$

holds, where $N-\mathcal{P}_{n_1,n_2,\ldots}$ is the number of particles in the condensed manifold. One thus arrives at

$$|\Psi\rangle = \sum_{n_1=0,n_2=0,\ldots} |N-\mathcal{P}_{n_1,n_2,\ldots},n_1,n_2,n_3\ldots\rangle C_{n_1,n_2,\ldots}, \tag{38b}$$

which is particle-number conserving and contact has been made with the exact eigenstate of the full Hamiltonian; see Sec. II C 1.

One should be aware that we are discussing here the wave function for very large N or, actually, even for $N\to\infty$. Whatever the total number of phonons in an unperturbed state is, N should be much larger. We have arguments to believe that the above is also very useful for finite values of N. The numerical results for the many-body quantities beyond mean field as well as the energy and density per particle seem to converge numerically already for finite and rather moderate values of N [12]. But for finite values of N one may argue that the total number of phonons in an unperturbed state could be larger than N. However, the contribution of unperturbed states $|N-\mathcal{P}_{n_1,n_2,\ldots},n_1,n_2,\ldots\rangle$ to an exact eigenstate falls off dramatically as the number of particles removed from the condensate manifold grows, i.e., as the total number of phonons in an unperturbed state grows. This is due to the fact that the full Hamiltonian contains only one- and two-particle operators and many operators are needed to describe the coupling of a low-lying exact eigenstate with a highly excited unperturbed state.

We are left with the calculation of the expansion coefficients $C_{n_1,n_2,\ldots}$ in Eq. (38b). These can be obtained from recursion relations. Starting from $\langle n_1,n_2,\ldots|c_i|\bar{0}\rangle = 0$ one finds [45]

$$C_{n_1,\ldots,n_i+1,\ldots} = -\sum_{j=1}\sqrt{\frac{n_j}{n_i+1}} f_{ij} C_{n_1,\ldots,n_j-1,\ldots}, \tag{39}$$

where f_{ij} is given as the determinant of the matrix $\boldsymbol{\Xi}_1\boldsymbol{\Xi}_1^\dagger$ with the ith column replaced by the column vector $(\boldsymbol{\Xi}_2^\dagger\boldsymbol{\Xi}_1)_{1j},(\boldsymbol{\Xi}_2^\dagger\boldsymbol{\Xi}_1)_{2j},\ldots$ divided by $\det(\boldsymbol{\Xi}_1\boldsymbol{\Xi}_1^\dagger)$.

If one wishes to compute equations analogous to Eq. (38b), but for excited states and not for the ground state, more involved recursion relations have to be used which can be found in the Appendix of [45].

Explicit examples for reconstructing the wave function are presented in the following sections.

IV. APPLICATION: THE HARMONIC INTERACTION MODEL

A. The model

To the knowledge of the authors, the only analytically solvable model of N interacting bosons in a trap is the harmonic interaction model (HIM). In this model the boson-boson interaction potential is harmonic and the bosons move in a harmonic trap. The model has been solved explicitly in the literature [46] and has served in several works either as a test for computational methods or for investigating new physics [12,47–52]. The model can be solved in any dimension, but for brevity we will investigate it here in 1D. As the model is analytically solvable, we will study it in the context of the infinite-particle limit to compare its results with those of the phonon Hamiltonian of Sec. III.

In a harmonic trap of frequency ω the HIM Hamiltonian reads

$$H = \sum_{i=1}^{N}\left(\frac{\hat{p}_i^2}{2}+\frac{\omega^2}{2}x_i^2\right)+\lambda_0\sum_{i<j}^{N}(x_i-x_j)^2. \tag{40a}$$

By introducing normal coordinates, this Hamiltonian becomes separable and hence solvable analytically. The exact ground-state wave function is a product of $N-1$ oscillators of frequency $\delta_N^2=\omega^2+2\lambda_0 N$ in their ground state and one oscillator with frequency ω describing the center-of-mass motion of the system [46].

To rewrite the above Hamiltonian in second quantization with the mean field as the unperturbed Hamiltonian, we first need the Fock operator, see Eqs. (2) and (3), which takes on the appearance

$$\hat{F} = \left(\frac{\hat{p}^2}{2}+\frac{\omega^2}{2}x^2\right)+\Lambda\int|\varphi_0(x')|^2(x-x')^2dx'. \tag{40b}$$

Solving the self-consistent eigenvalue equation $\hat{F}|\varphi_0\rangle = \mu_0|\varphi_0\rangle$ gives

$$\varphi_0(x) = \left(\frac{\delta}{\pi}\right)^{1/4} e^{(-\frac{\delta}{2}x^2)}, \qquad \delta^2=\omega^2+2\Lambda. \tag{40c}$$

Note that the frequency δ is identical to δ_{N-1} introduced above.

With the above one easily obtains the Fock operator and its eigenvalues μ_n explicitly:

$$\hat{F} = \left(\frac{\hat{p}^2}{2}+\frac{\delta^2}{2}x^2\right)+\frac{\Lambda}{2\delta}, \quad \mu_n = \left(n+\frac{1}{2}\right)\delta+\frac{\Lambda}{2\delta}, \tag{40d}$$

and it is also straightforward to compute the relevant matrix elements of the boson-boson interaction:

$$V_{0000} = \frac{1}{\delta}, \qquad V_{nn'00} = V_{0nn'0} = -\frac{\delta_{n1}\delta_{n'1}}{\delta}. \tag{40e}$$

All the quantities defining the phonon Hamiltonian (23) or equivalently (26) are now explicitly available and are given by

$(n,n' \geqslant 1)$

$$E_{\mathrm{MF}} = \frac{N}{2}\delta, \qquad C_E = E_{\mathrm{MF}} - \sum_{n=1}\frac{1}{2}\omega_n + \frac{\Lambda}{2\delta},$$
$$\omega_n = n\delta, \quad \gamma_{nn'} = -\frac{\delta_{n1}\delta_{n'1}}{2\delta}, \quad \tau_{nn'} = 0. \tag{40f}$$

It is seen that the phonon Hamiltonian is rather simple as only the first excited orbital φ_1 couples to the condensed manifold. This greatly simplifies finding the solution of this Hamiltonian.

B. The properties of the phonon Hamiltonian

With the quantities entering the phonon Hamiltonian found above, the eigenvalue equation (32) becomes particularly simple as the matrix to be diagonalized is already diagonal. This implies that $\mathbf{Z} = \mathbf{1}$ and all eigenvalues except of $\bar{\omega}_1$ are not affected, i.e., $\bar{\omega}_n = \delta$. The new frequency $\bar{\omega}_1$ is determined from $\delta^{\frac{1}{2}}(\delta + 4\gamma_{11})\delta^{\frac{1}{2}} = \bar{\omega}_1^2$ which readily gives

$$\bar{\omega}_1 = \omega, \tag{41}$$

which is nothing but the frequency of the bare trap potential. Clearly, this $n = 1$ mode describes the center-of-mass motion of the system.

Now, one can calculate the transformation between the mean-field operators b_n and the c_n which make the Hamiltonian diagonal. From Eq. (31), one finds $J_{11} = (\omega/\delta)^{\frac{1}{2}}$ and all other elements are $J_{nn'} = \delta_{nn'}$. The transformation matrix readily follows from Eq. (30):

$$(\Xi_1)_{11} = \frac{\omega+\delta}{2\sqrt{\omega\delta}}, \quad (\Xi_1)_{nn'} = \delta_{nn'}, \tag{42}$$
$$(\Xi_2)_{11} = \frac{\omega-\delta}{2\sqrt{\omega\delta}}, \quad (\Xi_2)_{nn'} = 0.$$

In other words, the phonon destruction operators are given by $c_1 = (\frac{\omega+\delta}{2\sqrt{\omega\delta}})b_1 + (\frac{\omega-\delta}{2\sqrt{\omega\delta}})b_1^\dagger$ and all other $c_n = b_n$.

We are now in the position to compute all the quantities introduced. Let us start with the energy. The mean-field energy $E_{\mathrm{MF}} = \frac{N}{2}\delta$ is, of course, the same as in the analytic solution of the model [46]. The general expression for the correlation energy E_c in the phonon Hamiltonian can be found in Eq. (35). In the present example it takes on the following appearance:

$$E_c = -\frac{\Lambda}{2\delta} - \frac{1}{2}(\omega - \delta). \tag{43a}$$

The analytically exact result for any N is known to be $E_c = \frac{N}{2}\delta_{N-1} - \frac{N-1}{2}\delta_N - \frac{\omega}{2}$, see [46], and we would like to compare the two expressions for large N. For that purpose we expand the quantity $(N-1)\delta_N$ for N particles to give the corresponding quantity for $N-1$ particles: $(N-1)\delta_N = (N-1)\delta_{N-1} + \Lambda/\delta_{N-1} + O(1/N)$. Inserting into the analytic expression immediately provides the identical result found in Eq. (43a) for the phonon Hamiltonian.

For completeness, we also study the correlation energy for small coupling strength Λ. Expanding δ in a Taylor series in Λ gives $\delta = \omega + \frac{\Lambda}{\omega} - \frac{\Lambda^2}{4\omega^3} + \cdots$. Inserted into Eq. (43a) leads to $E_c = \frac{\Lambda^2}{4\omega^3}$. Of course, this result is identical to that obtained with the perturbation expression (15) in the limit of infinite N.

We now turn to the overlap of the mean-field and exact ground-state wave functions. Using the general Eq. (33) for this overlap, one readily obtains with the aid of the elements in Eq. (42)

$$S = [\det(\Xi_1)]^{-\frac{1}{2}} = 2^{\frac{1}{2}}\frac{(\delta\omega)^{\frac{1}{4}}}{(\delta+\omega)^{\frac{1}{2}}}. \tag{43b}$$

The analytical solution for the overlap of the wave functions is provided for large N in [12] for all dimensions. In 1D one obtains directly from Eq. (7a) in the latter reference $S = 2^{\frac{1}{2}}\frac{(1+2\Lambda/\omega^2)^{\frac{1}{8}}}{[1+\sqrt{(1+2\Lambda/\omega^2)}]^{\frac{1}{2}}}$. Straightforward manipulations of this expression give a result identical to that in Eq. (43b).

Next, we investigate the depletion $D(\Lambda)$ of the ground state. The corresponding general expression derived for the phonon Hamiltonian has been derived in Sec. III C 2. Using Eq. (34) and the quantities for the HIM in (42), one immediately obtains the simple expression

$$D = \mathrm{Tr}[\Xi_2\Xi_2^\dagger] = \frac{1}{4}\frac{(\delta-\omega)^2}{\delta\omega}. \tag{43c}$$

The exact depletion and natural orbitals for HIM can be obtained analytically from the eigenvalues and eigenvectors of the one-body reduced density matrix [53,54]. For large N the most occupied natural orbital becomes identical with the mean-field orbital (see Sec. II C 5) and hence the weight of this orbital provides $\rho_{00} = N - D$. The expression obtained is lengthy and its Taylor expansion in powers of $1/N$ gives exactly the same result as in Eq. (43c).

C. The reconstruction of the wave function

By comparing with the analytically derived solutions of the HIM, it has been seen that the phonon Hamiltonian has provided exact results for the energy, overlap with the mean-field wave function, and depletion of the ground state in the limit $N \to \infty$. The ultimate goal is to demonstrate that the full particle-conserving wave function of the problem can be reconstructed from the non-particle-conserving solution of the phonon Hamiltonian.

The general idea and procedure of the reconstruction are discussed in Sec. III D. Since in the HIM we have shown that there is only a single active phonon mode available, we can formulate the problem more compactly using only this mode and the condensed manifold.

For large but finite N, we thus write the self-explanatory equation

$$|\Psi\rangle = \sum_{n_1=0}|N-n_1,n_1\rangle C_{n_1},$$
$$C_{n_1} = \langle n_1|\bar{0}\rangle. \tag{44a}$$

To proceed we remind the reader that C_0 is nothing but the overlap explicitly given in Eq. (43b), and that C_1 as well as all C_{n_1} with an odd number of phonons in this mode vanish because of symmetry. One has to determine the $C_2, C_4, \ldots$ for the even occupation numbers and this is accomplished with the recursion relation

$$C_{n_1+1} = -\sqrt{\frac{n_1}{n_1+1}}f_{11}C_{n_1-1}. \tag{44b}$$

Since C_0 is known, the only quantity to be determined in order to evaluate the wave function is f_{11}.

One can determine the quantity f_{11} by the procedure explained in Sec. III. We would like, however, to proceed differently. The sum over all the squared coefficients is, of course, unity: $\sum_{n_1=0} |C_{n_1}|^2 = 1$. From the recursion relation one readily sees for $m = 1,2,\ldots$ that

$$C_{2m} = (-1)^m \sqrt{\frac{1 \times 3 \times \ldots (2m-1)}{2 \times 4 \times \ldots (2m)}} f_{11}^m C_0 \tag{44c}$$

and we identify the sum of squares to be the Taylor expansion of

$$1 = \left(1 - f_{11}^2\right)^{-\frac{1}{2}} |C_0|^2.$$

Using the explicit HIM expression in Eq. (43b) for C_0, one arrives at the following simple expression for the missing quantity:

$$f_{11} = \frac{\omega - \delta}{\omega + \delta}. \tag{44d}$$

This completes the reconstruction of the wave function.

In Fig. 1 the expansion coefficients C_{2m} of the many-body wave function are shown for $\Lambda = 100$ computed with the above equations. Note that the overlap S discussed in Sec. IV B is provided by the first coefficient C_0. It is clearly seen that the wave function is rather complex although we have learned that the energy and density per particle are exactly determined by the respective mean-field quantities. In the representation of Fig. 1, the mean-field wave function would consist of a single bar C_0 of unity height. As all observables of a system are determined by the wave function, there are many properties which will deviate strongly from the respective mean-field ones. Examples have been given in [12,23,24,44].

It is rather cumbersome to compute the exact analytically known wave function in the basis of the mean-field orbitals

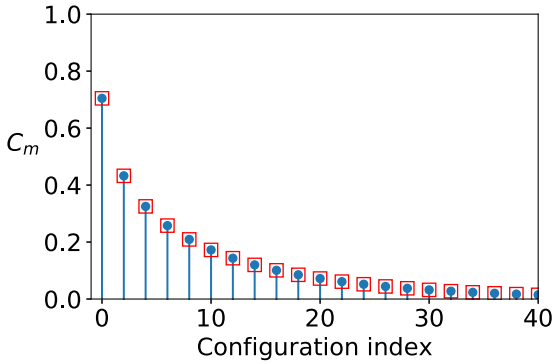

FIG. 1. The ground-state wave function of the HIM. The red squares show the value of the reconstructed wave function using the results of the phonon Hamiltonian. Shown are the coefficient C_{n_1} of the wave function computed employing the analytic formula (44c). Note that the coefficient C_0 is the overlap of the mean-field and exact wave function. The blue dots show the same coefficients computed numerically for the *full* Hamiltonian (40a) using the MCTDHB method for $N = 10^7$ bosons. The values of the coefficients do not change if N is lowered to $N = 10^6$. In all calculations the value of $\Lambda = 100$ has been used.

as done here. To have a comparison with the reconstructed wave function, we have performed numerical calculations employing the variational multiconfigurational time-dependent Hartree for bosons (MCTDHB) method [55,56] in which the ground state is found by imaginary-time propagation. The MCTDHB is a well-established method in the literature [57]. In principle, it is a numerically exact method [52], but for large boson numbers it can only be solved approximately as the number of boson Fock states explodes. The method has been tested for HIM [12,52]. The expansion coefficients C_{2m} computed numerically for $N = 10^7$ bosons are shown in Fig. 1 for the same coupling strength as used for the reconstructed wave function. It is clearly seen that the reconstructed wave function excellently reproduces the numerically determined particle-conserving wave function.

Two remarks are in order. Because the coupling strength $\Lambda = \lambda_0(N-1)$ is held constant as $N \to \infty$, it is obvious that the parameter λ_0 measuring the interaction between two bosons is infinitesimally small. In this respect, even very large values of Λ are easily achievable. We have already mentioned that for a given value of Λ, relevant properties like the correlation energy, depletion, and elements of the density matrix do not change with varying N provided that N is large enough. This applies also to the wave function itself. The larger the interaction strength Λ, the larger is usually the value of N needed. This explains why one can reconstruct the wave function for a finite but large N with the aid of the calculation starting from the phonon Hamiltonian which has been derived for $N \to \infty$.

V. APPLICATION: INTERACTING BOSONS ON A FINITE RING

A. The model

There has been considerable interest in studying interacting bosons on a ring. Originally, most of the works concentrated on the thermodynamic limit in which the length of the ring goes to infinity. Here, the inconsistencies found in GP theory [3,17] were removed by the theory of Bogoliubov [3,27]. Using the Bethe ansatz [58], Lieb and Liniger [59] derived a system of $N-1$ coupled transcendental equations for the exact N-particle ground state of a finite ring and contact interaction. They solved this system explicitly for two particles, but then passed to the thermodynamic limit and showed that the whole system of coupled transcendental equations can be approximated by a single Fredholm integral equation of the second kind. They solved this integral equation and demonstrated that for weak interactions Bogoliubov's theory agrees well with this solution, and for strong interactions the solution approaches that of the Tonks-Girardeau gas in the thermodynamic limit [60]. For contact interaction the Lieb and Liniger solution can be considered as the essentially exact solution of the thermodynamic limit.

In this section we are interested in solving the problem of bosons on a ring of finite length in the infinite-particle limit employing the contact boson-boson interaction potential. Here, as $N \to \infty$, the coupling strength Λ is kept constant. As mentioned above, Lieb and Liniger derived the system of coupled equations for finite N and length of the ring,

and solved them for two bosons on the ring. Their coupled transcendental equations are difficult to solve. It took more than 30 years until Muga and Snider solved the spectrum of the three-particle problem [61]. A few years later, Sakmann *et al.* [62] succeeded in computing the exact ground state for up to 50 bosons. It was found that there is still a substantial dependence on the length of the ring and on the number of bosons.

By writing $x = \phi L/2\pi$, where L is the length of the ring, one can transfer the many-boson Hamiltonian (1) with contact interaction to angular coordinates. After multiplication with L^2 one obtains

$$H = -\sum_{i=1}^{N} \frac{\partial^2}{\partial \phi_i^2} + \lambda_0 L \sum_{j>i} \delta(\phi_i - \phi_j). \tag{45}$$

To obtain the correct energies, one has to divide the eigenvalues of this Hamiltonian by L^2.

Choosing the mean-field potential to be symmetry preserving, the orbitals are eigenfunctions of the angular momentum operator perpendicular to the ring. The Fock operator and its solutions, see Eq. (3), take on the expressions

$$\hat{F} = -\frac{\partial^2}{\partial \phi^2} + \frac{\Lambda L}{2\pi}, \quad \varphi_s = \frac{e^{is\phi}}{\sqrt{2\pi}}, \quad \mu_s = s^2 + \frac{\Lambda L}{2\pi}. \tag{46}$$

The orbitals φ_s with the quantum numbers $s = 0, \pm 1, \pm 2, \ldots$ are normalized in the interval $[-\frac{\pi}{2}, \frac{\pi}{2}]$. The orbital φ_0 is, as usual, the orbital of the condensate manifold.

To continue, one needs the four-index integrals computed in the above basis of mean-field orbitals:

$$V_{ijkl} = \frac{L}{2\pi} \delta_{i+j=k+l}, \tag{47}$$

where the δ symbol stands for the conservation of the angular momentum perpendicular to the ring.

This completes the calculation of the Hamiltonian (5) in second quantization and we are in the position to move on to the phonon Hamiltonian in Eq. (23) or, equivalently, (26). All the quantities entering the phonon Hamiltonian are listed below for $s, s' \neq 0$:

$$\begin{aligned} E_{\mathrm{MF}} &= \frac{NL\Lambda}{4\pi}, \quad C_E = E_{\mathrm{MF}} - \sum_s \frac{1}{2}\omega_s - \sum_s \frac{\Lambda L}{4\pi}, \\ \omega_s &= s^2, \quad \gamma_{s,s'} = \frac{\Lambda L}{8\pi}(\delta_{s,-s'} + \delta_{s,s'}), \\ \tau_{s,s'} &= \frac{\Lambda L}{8\pi}(\delta_{s,-s'} - \delta_{s,s'}). \end{aligned} \tag{48}$$

As in the former application to HIM, the quantity C_E contains divergent sums which are, however, exactly made finite by contributions from the ground-state energy of the Hamiltonian. See also below. The divergence comes from the fact that one has an infinite number of phonon modes whose zero-point energy is infinite. In numerical applications, one can first consider a large but finite number of modes and later increase this number until convergence is achieved.

B. The diagonalization of the phonon Hamiltonian

In the previous application (HIM) the matrix to be diagonalized was found to be diagonal and hence the solution was straightforward. In the present application the matrix $(\boldsymbol{\omega} - 4\boldsymbol{\tau})^{\frac{1}{2}}(\boldsymbol{\omega} + 4\boldsymbol{\gamma})(\boldsymbol{\omega} - 4\boldsymbol{\tau})^{\frac{1}{2}}$ to be diagonalized is not *a priori* seen to be diagonal and the problem is more involved. Fortunately, this matrix, which we denote $\mathbf{M}$, has a block-diagonal structure of 2×2 matrices $\mathbf{M}_s$, $s = 1,2,\ldots$, along the diagonal. Each 2×2 block consists of elements $m_{s,s}, m_{s,-s}, m_{-s,s}, m_{-s,-s}$ and can, of course, be easily diagonalized.

To construct a 2×2 block $\mathbf{M}_s$ we first compute the individual components

$$(\boldsymbol{\omega} - 4\boldsymbol{\tau})_s = \begin{pmatrix} s^2 + \frac{\Lambda L}{2\pi} & -\frac{\Lambda L}{2\pi} \\ -\frac{\Lambda L}{2\pi} & s^2 + \frac{\Lambda L}{2\pi} \end{pmatrix},$$

$$(\boldsymbol{\omega} + 4\boldsymbol{\gamma})_s = \begin{pmatrix} s^2 + \frac{\Lambda L}{2\pi} & \frac{\Lambda L}{2\pi} \\ \frac{\Lambda L}{2\pi} & s^2 + \frac{\Lambda L}{2\pi} \end{pmatrix},$$

which are nondiagonal. To compute the square root of a general Hermitian matrix $\mathbf{A}$, one has to first diagonalize it, i.e., solve for $\mathbf{AS} = \mathbf{S}\boldsymbol{\epsilon}$, where $\mathbf{S}$ is the unitary eigenvector and $\boldsymbol{\epsilon}$ the diagonal eigenvalue matrices. The square root then is $\mathbf{A}^{\frac{1}{2}} = \mathbf{S}\boldsymbol{\epsilon}^{\frac{1}{2}}\mathbf{S}^{\dagger}$. Interestingly, although all involved 2×2 components of $\mathbf{M}_s$ are not diagonal, their product is, and we find

$$\mathbf{M}_s = \begin{pmatrix} s^2(s^2 + \frac{\Lambda L}{\pi}) & 0 \\ 0 & s^2(s^2 + \frac{\Lambda L}{\pi}) \end{pmatrix}.$$

One sees again that, as in HIM, the matrix $\mathbf{Z} = \mathbf{1}$. The eigenvalues of $\mathbf{M}$ are simply given by

$$\bar{\omega}_s^2 = \bar{\omega}_{-s}^2 = s^2\left(s^2 + \frac{\Lambda L}{\pi}\right) \tag{49}$$

and seen to come in doubly degenerate pairs.

The matrix $\mathbf{J}$ in Eq. (31) which we need to compute the transformation from the bare operators b_s to the new ("dressed") phonon operators c_s is, however, nondiagonal. Nevertheless, the resulting transformation, computed using Eqs. (30) and (28), does have a rather compact structure:

$$\begin{aligned} (\boldsymbol{\Xi}_1)_s &= \frac{1}{2}\begin{pmatrix} \alpha_s^+ & 0 \\ 0 & \alpha_s^+ \end{pmatrix}, \quad (\boldsymbol{\Xi}_2)_s = \frac{1}{2}\begin{pmatrix} 0 & \alpha_s^- \\ \alpha_s^- & 0 \end{pmatrix}, \\ \alpha_s^{\pm} &= |s|^{-\frac{1}{2}}\left(s^2 + \frac{\Lambda L}{\pi}\right)^{\frac{1}{4}} \pm |s|^{\frac{1}{2}}\left(s^2 + \frac{\Lambda L}{\pi}\right)^{-\frac{1}{4}}. \end{aligned} \tag{50}$$

We are now in the position to calculate the properties of interest. This is done in the next subsection.

C. The properties of the phonon Hamiltonian

1. The correlation energy

The general expression for the correlation energy computed with the phonon Hamiltonian is provided in Eq. (35). To compute this quantity one needs only the dressed frequencies $\bar{\omega}_s$ and not the transformation matrix $\boldsymbol{\Xi}$ itself and this is the reason why we first study the correlation energy here. This

energy is simply given by

$$E_c = -\sum_{s=1}\left\{s\left[\left(s^2+\frac{\Lambda L}{\pi}\right)^{\frac{1}{2}}-s\right]-\frac{\Lambda L}{2\pi}\right\}, \tag{51a}$$

where we have made use of the symmetry $s \leftrightarrow -s$, see, e.g., Eq. (49), and reduced the sum over all values of $s \neq 0$ to positive values $s \geqslant 1$ only.

To better understand how the above infinite sum converges, one can rewrite the expression inside the braces as $s^2[(1+\frac{\Lambda L}{\pi s^2})^{\frac{1}{2}}-(1+\frac{\Lambda L}{2\pi s^2})]$. Independently of how large ΛL is, from large enough values of s^2 on, this term will behave as s^{-2} assuring convergence (see also below).

Let us now discuss the behavior of the correlation energy for small ΛL. For that purpose one can just expand $(1+\frac{\Lambda L}{\pi s^2})^{\frac{1}{2}}$ in a Taylor series in the small quantity $\frac{\Lambda L}{\pi s^2}$ and obtain $1+\frac{1}{2}\frac{\Lambda L}{\pi s^2}-\frac{1}{8}(\frac{\Lambda L}{\pi s^2})^2+\cdots$. The first two terms in this expansion directly compensate the last two terms inside the braces, and we are left with

$$E_c = \frac{1}{8}\left(\frac{\Lambda L}{\pi}\right)^2\sum_{s=1}^{\infty}\frac{1}{s^2} = \frac{\Lambda^2 L^2}{48}, \tag{51b}$$

as the leading term.

In the absence of an exact solution of the problem of bosons on a ring, we compare this result with that obtained employing the perturbation theory developed in Sec. II B for the full many-body Hamiltonian (5). With the eigenvalues of the Fock operator given in Eq. (46) and the four-index integrals in Eq. (47), one can evaluate the correlation energy in second order which is provided in Eq. (15):

$$E_c = \frac{\Lambda^2}{2}\frac{N}{N-1}\sum_{s,s'}\frac{\delta_{s,-s'}\left(\frac{L}{2\pi}\right)^2}{s^2+s'^2} = \frac{N}{N-1}\frac{\Lambda^2 L^2}{48}. \tag{51c}$$

Obviously, for large N the phonon Hamiltonian leads to exactly the same result as does the full Hamiltonian.

The correlation energy as a function of $L\Lambda$ has been computed numerically with Eq. (51a). The results are shown in the upper panel of Fig. 2 as a function of ΛL. This energy is seen to grow monotonically with the interaction strength and the length of the ring and any finite value can be achieved.

2. The depletion of the condensate

According to Sec. III C 2 the depletion of the condensate computed with the phonon Hamiltonian is given by $D = \mathrm{Tr}[\Xi_2\Xi_2^\dagger]$. The elements of the transformation matrix are collected in Eq. (50) and it is seen that the product $\Xi_2\Xi_2^\dagger$ is a diagonal matrix with elements $(\alpha_s^-)^2/4$ along the diagonal. Correspondingly, after some simple manipulations as done above for the correlation energy, the depletion takes on the appearance

$$D = \frac{1}{2}\sum_{s=1}^{\infty}\left[\left(1+\frac{\Lambda L}{\pi s^2}\right)^{\frac{1}{2}}+\left(1+\frac{\Lambda L}{\pi s^2}\right)^{-\frac{1}{2}}-2\right]. \tag{52a}$$

Clearly, the above sum is well behaved and converges rather rapidly.

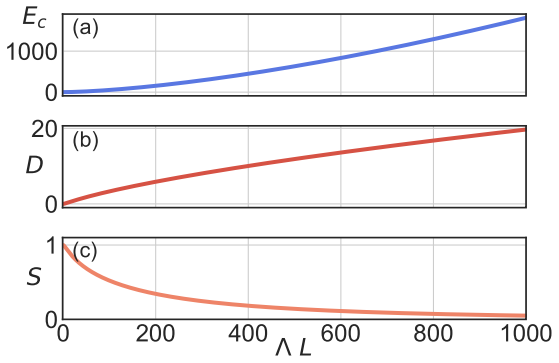

FIG. 2. Results of numerical calculations for bosons on a ring in the infinite-particle limit. The results are shown as a function of ΛL, where L is the length of the ring and Λ is the interaction strength. Upper panel: Correlation energy computed using the analytic formula (51a). Middle panel: Depletion of the condensate computed using the analytic formula (52a). Lower panel: Overlap of the mean-field and exact wave function computed using the analytic formula (53a). All quantities are dimensionless.

For small values of ΛL one can expand the terms in Eq. (52a) in powers of $\frac{\Lambda L}{\pi s^2}$ and readily obtain

$$D = \frac{\Lambda^2 L^2}{8\pi^2}\sum_{s=1}^{\infty}\frac{1}{s^4} = \frac{\pi^2\Lambda^2 L^2}{8\times 90}. \tag{52b}$$

To compare with the perturbation expansion of the depletion derived for the full many-body Hamiltonian, one can resort to Eqs. (14) and (12). In the present context the leading term in the expansion reads

$$D = \frac{\Lambda^2 N}{N-1}\sum_{s,s'}\frac{\delta_{s,-s'}\left(\frac{L}{2\pi}\right)^2}{(s^2+s'^2)^2} = \frac{N}{N-1}\frac{\pi^2\Lambda^2 L^2}{8\times 90}, \tag{52c}$$

verifying again the result obtained for the phonon Hamiltonian.

It is interesting to investigate the depletion as a function of $L\Lambda$. The results of the computation using the analytic expression (52a) are depicted in Fig. 2. The depletion, i.e., the number of bosons outside the condensed manifold, grows monotonically with $L\Lambda$. It should be remembered that each of the bosons outside the condensate manifold interacts with all the infinitely many bosons in the condensed manifold and this makes the wave function highly complex and very different from the mean-field one.

3. The overlap of the mean-field and exact wave functions

In the framework of the phonon Hamiltonian the overlap between the exact and mean-field wave functions has been shown to be given by $S = [\det(\Xi_1)]^{-\frac{1}{2}}$, and since the matrix Ξ_1 is diagonal for the problem at hand, the calculation of its determinant is simple. Employing Eq. (50) and noticing that the elements of this matrix are the same for positive and negative values of the quantum number s, one readily obtains

$$S = \prod_{s=1}^{\infty}\frac{2}{\left[\left(1+\frac{\Lambda L}{\pi s^2}\right)^{\frac{1}{4}}+\left(1+\frac{\Lambda L}{\pi s^2}\right)^{-\frac{1}{4}}\right]}. \tag{53a}$$

This product form is convergent. For any finite value of $\frac{\Lambda L}{\pi}$, one can write this product as a quotient of products up to some finite value of s, where $s \gg \frac{\Lambda L}{\pi}$, times a convergent product; see below.

For small values of the interaction strength, we can Taylor expand the above terms in the denominator and retain the leading term. This results in the following expression for $\Lambda L \to 0$:

$$S = \prod_{s=1}^{\infty}\left[1 - \frac{1}{32}\left(\frac{\Lambda L}{\pi s^2}\right)^2\right] \tag{53b}$$
$$= 1 - \frac{\Lambda^2 L^2}{32\pi^2}\sum_{s=1}^{\infty}\frac{1}{s^4} = 1 - \frac{\pi^2\Lambda^2 L^2}{32\times 90}.$$

To compare with the perturbation theoretical result of the full many-body Hamiltonian (1) or, equivalently (5), we return to Eqs. (12) and (14) and similarly to what was found above for the depletion D we find

$$S = 1 - \frac{N}{N-1}\frac{\pi^2\Lambda^2 L^2}{32\times 90}, \tag{53c}$$

in agreement with the result determined in Eq. (53b) within the framework of the phonon Hamiltonian.

The overlap S computed with the aid of Eq. (53a) is plotted in Fig. 2 as a function of ΛL. The overlap falls off monotonically as either the length of the ring or the interaction strength grows. It can be made to essentially vanish.

4. The reduced one-body density matrix

The reduced one-body density matrix takes on the appearance $\boldsymbol{\rho} = \boldsymbol{\Xi}_2^\dagger \boldsymbol{\Xi}_2$; see Sec. III C 4. For interacting bosons on a ring the matrix $\boldsymbol{\Xi}_2$ is provided explicitly in Eq. (50) and is nondiagonal, but the product $\boldsymbol{\Xi}_2^\dagger \boldsymbol{\Xi}_2$ is diagonal. The result is

$$\rho_{ss'} = \delta_{ss'}\left[\left(1 + \frac{\Lambda L}{\pi s^2}\right)^{\frac{1}{4}} - \left(1 + \frac{\Lambda L}{\pi s^2}\right)^{-\frac{1}{4}}\right]. \tag{54a}$$

From this expression the leading term in Λ is easily determined to give

$$\rho_{ss'} = \delta_{ss'}\left(\frac{\Lambda L}{4\pi s^2}\right)^2. \tag{54b}$$

According to the perturbation theory of the full Hamiltonian, the elements of the reduced matrix read [see Eq. (17)]

$$\rho_{ss'} = \Lambda^2\frac{N}{(N-1)}\sum_k \frac{\delta_{-k,s}\delta_{-k,s'}\left(\frac{L}{2\pi}\right)^2}{(s^2+k^2)(s'^2+k^2)}$$
$$= \delta_{ss'}\frac{N}{N-1}\left(\frac{\Lambda L}{4\pi s^2}\right)^2. \tag{54c}$$

D. Reconstruction of the wave function in the infinite-particle limit

In contrast to the HIM problem solved in Sec. IV where a single phonon mode has been found to be active, in the case of bosons on a ring the ground state contains infinitely many active phonon modes specified by $s = \pm 1, \pm 2, \ldots$. The method introduced in Sec. III D to reconstruct the number-conserving eigenstate of the full many-body Hamiltonian is also valid here, but we have to decide which components of the wave function are to be explicitly computed. From the general perturbation theory starting with the mean-field Hamiltonian it is clear now that the most important contributions are expected from the doubly excited boson configurations. Because of that and also as a demonstration of the reconstruction procedure, we will first determine the respective contributions to the wave function.

The exact and mean-field ground states, $|\bar{0}\rangle$ and $|0\rangle$, have a total angular momentum of 0. Consequently, we can only expect contributions from excited configurations which do not alter the angular momentum. Singly excited configurations obviously change the angular momentum and hence do not contribute. The lowest type of excitations which do not alter the angular momentum are the doubly excited configurations $|1_s, 1_{-s}\rangle = b_s^\dagger b_{-s}^\dagger|0\rangle$. Their contribution to the ground state is, in the nomenclature of Sec. III D,

$$C_{1_s,1_{-s}} = \langle 0|b_{-s}b_s|\bar{0}\rangle. \tag{55}$$

To evaluate the above quantity, we start with the identity

$$\langle 0|b_{-s}c_s|\bar{0}\rangle = 0, \tag{56}$$

where the c_s are the operators for the dressed phonons diagonalizing the phonon Hamiltonian; see Sec. III B.

To proceed, one has to make use of the relationship (28) between the mean-field and dressed operators. For bosons on a ring the transformation matrix is given in Eq. (50). The explicit relationship

$$c_s = \tfrac{1}{2}\alpha_s^+ b_s + \tfrac{1}{2}\alpha_s^- b_{-s}^\dagger \tag{57}$$

is of interest by itself as it reflects the angular momentum character of the operators. In this equation s can be positive or negative.

Inserting the latter into the identity (56) and keeping in mind that b_s and $b_{-s}^\dagger$ commute and the creation operators when operating to the left annihilate the mean-field ground state, one finds

$$C_{1_s,1_{-s}} = -\frac{\alpha_s^-}{\alpha_s^+}C_0 = -\frac{\left(1+\frac{\Lambda L}{\pi s^2}\right)^{\frac{1}{4}} - \left(1+\frac{\Lambda L}{\pi s^2}\right)^{-\frac{1}{4}}}{\left(1+\frac{\Lambda L}{\pi s^2}\right)^{\frac{1}{4}} + \left(1+\frac{\Lambda L}{\pi s^2}\right)^{-\frac{1}{4}}}C_0. \tag{58a}$$

The quantity C_0 is just the overlap $S = \langle 0|\bar{0}\rangle$ which can be found in Eq. (53a). From the above it is evident that the larger the angular momentum of the mode, the less important this mode is for the ground-state wave function.

To make contact with perturbation theory of the full Hamiltonian, one may expand the expression above for small values of Λ and obtain $C_{1_s,1_{-s}} = -\frac{\Lambda L}{4\pi s^2}$. Using the correction to the state in first order in Eq. (10), and taking care that the Fock states appear there twice, one finds

$$|\tilde{\Psi}^{(1)}\rangle = -\frac{\Lambda L}{4\pi}\sqrt{\frac{N}{(N-1)}}\sum_{s=1}\frac{1}{s^2}|N-2, 1_s, 1_{-s}\rangle, \tag{58b}$$

which for large N reproduces the result reconstructed from the phonon Hamiltonian.

We now move to the next higher classes of excitations. From the identity $\langle 0|b_{s''}b_{s'}c_s|\bar{0}\rangle = 0$ and Eq. (57) one readily notices that all triple excitations do not contribute to the ground wave function. The contribution of the next class of excitations can be determined starting from the identity $\langle 0|b_{s'''}b_{s''}b_{s'}c_s|\bar{0}\rangle = 0$. Keeping in mind that the total angular momentum $s + s' + s'' + s'''$ equals zero, we find for the nonvanishing contributions

$$C_{1_s,1_{-s},1_{s'},1_{-s'}} = -\left(\frac{\alpha^-_{s'}}{\alpha^+_{s'}}\right)C_{1_s,1_{-s}},$$

$$C_{2_s,2_{-s}} = -\sqrt{2}\left(\frac{\alpha^-_{s'}}{\alpha^+_{s'}}\right)C_{1_s,1_{-s}}. \tag{58c}$$

Following the reconstruction scheme detailed in Sec. III D, we are now in the position to express the particle-number-conserving wave function as

$$|\Psi\rangle/C_0 = |N\rangle - \sum_{s=1}\left(\frac{\alpha^-_s}{\alpha^+_s}\right)|N-2,1_s,1_{-s}\rangle + \sum_{s,s'\neq s}\left(\frac{\alpha^-_s}{\alpha^+_s}\right)\left(\frac{\alpha^-_{s'}}{\alpha^+_{s'}}\right)|N-4,1_s,1_{-s},1_{s'},1_{-s'}\rangle + \sqrt{2}\sum_{s=1}\left(\frac{\alpha^-_s}{\alpha^+_s}\right)^2|N-4,2_s,2_{-s}\rangle + \cdots. \tag{59}$$

We mention again that this expression is formally correct for $N \to \infty$, but in practice also for finite and large values of N. If ΛL is small, the values of N can be rather small for the above wave function to be accurate as long as $\frac{N}{N-1}$ is sufficiently close to 1. The larger the interaction strength becomes, the larger N must be for the wave function in (59) to be accurate.

VI. CONCLUSIONS

The mean-field potential of a general Hamiltonian of bosons in a trap interacting by a two-body potential is derived as usual by minimizing the energy expectation value in the mean-field ansatz. This allows one to formulate the second-quantized Hamiltonian in the basis of the mean-field Fock operator as done before [9,10,12]. For several classes of problems it is known that the mean-field reproduces the exact energy and density per particle correctly for $N \to \infty$. Indeed, with the formulation of the Hamiltonian in the mean-field basis one generally finds that this statement is correct, making this Hamiltonian particularly suitable to describe trapped boson systems. In this formulation, the perturbation theory starts with the mean-field Hamiltonian as the unperturbed Hamiltonian and the effective boson-boson interaction becomes the residual interaction left beyond mean field. For several relevant properties of the Hamiltonian as well as for its eigenstates the leading term in the perturbation expansion in the interaction strength Λ is given here. The only explicit dependence of these terms on the particle number N is found to be via the factor $\frac{N}{N-1}$. Clearly, all extensive parts of the quantities are thus collected in the mean-field part of these quantities, and one just investigates by the theory the fluctuations beyond mean field.

In the infinite-particle limit $N \to \infty$ keeping the interaction strength Λ fixed, one can simplify the derived full Hamiltonian in the spirit of Bogoliubov by collecting all destruction and creation operators which describe the condensate manifold and replacing each of them with $\sqrt{N}$. Bogoliubov has studied the thermodynamic limit of homogeneous systems which is, of course, a very different problem than ours. Ours is more related to the extension of Bogoliubov's theory by Fetter [30], which is, however, a non-particle-number-conserving theory. Our resulting simplified Hamiltonian is found to be particle-number conserving and is invariant to Gardiner's corrections [29] introduced to make Bogoliubov's theory particle-number conserving. The reason behind this invariance is the representation of the full Hamiltonian in the basis of the mean field.

This simplified Hamiltonian has been mapped on the structure of a Hamiltonian describing a typical system of coupled phonons which includes the interaction of the phonons through potential as well as through kinetic energy coupling. This Hamiltonian is called the phonon Hamiltonian. The mean-field destruction and creation operators are for bosons outside the condensed manifold and at the same time also for the coupled phonons. The phonon Hamiltonian can be brought to diagonal form by a linear transformation Ξ mixing the destruction and creation operators and giving rise to an eigenvalue equation. Physical properties computed with the phonon Hamiltonian are discussed and explicitly expressed by elements of this transformation matrix. By transforming back the solutions of the phonon Hamiltonian to their representation by the Fock states of the mean field and employing recursion relations, one can reconstruct the particle-conserving wave function of the full Hamiltonian, which we consider an important result. It is clear that this wave function is usually very different from the mean-field one. The depletion of the condensate is a constant for a large enough N, and this number of bosons outside the condensed manifold interacts with all the many or even infinite number of bosons in the condensed manifold. This makes the full wave function of the system very complex, sometimes of vanishing similarity to the mean-field one. Since the wave function determines all the observables of the system, it is clear that the true many-body character of the system is not to be looked for in the total energy or total density which are mean-field properties of the system. Other quantities, such as variances of various observables and correlation functions, reflect much better the many-body character of bosonic systems with many particles [12,23,24].

Two applications are discussed in some detail. In the first application the trap as well as the boson-boson interaction are harmonic (HIM). This model has been solved analytically in the literature [46] and thus the results found here using the phonon Hamiltonian can be tested. We find that the results of the phonon Hamiltonian are indeed exact in the infinite-particle limit. In this limit, we find that only a single phonon mode is active and this mode describes the center-of-mass motion of the system. The wave function of the HIM has been reconstructed from the phonon results and found to be rather involved. It coincides with accurate numerical calculations done on the full Hamiltonian.

In the second application we studied interacting bosons on a ring of a finite length L. Although this problem is much more complicated than the HIM, the phonon Hamiltonian could be

solved in *closed form*. All the properties investigated as well as the reconstructed wave function exhibit an interesting behavior as a function of ΛL. The wave function, in particular, is very complex and has typically little in common with the mean-field one. There is no exact solution expressed in closed form known in the literature for this problem and many particles. In order to have a comparison with exact results of the full Hamiltonian, we compare with the leading terms in ΛL obtained with the derived perturbation theory of the full Hamiltonian. In the limit of infinite particles, the two sets of results are identical as expected.

There are new physical results and also technical advances reported in this work. It is demonstrated that it is advantageous to express the full many-body Hamiltonian in the basis of the mean-field creation and annihilation operators. Perturbation theory formulated in this way, i.e., by using the mean-field as the unperturbed Hamiltonian, shows only a weak dependence of the wave function and other physical properties of interest on the number of bosons. The phonon Hamiltonian obtained following the Bogoliubov approach is shown to be *a priori* particle-number conserving when formulated in the mean-field basis and there is no need for corrections. Most importantly, the particle-number-conserving wave function of the system could be reconstructed, which is a completely new result. Having the wave function allows one to compute all desired properties of the system. Several properties of interest are discussed explicitly. It is seen that for generic trap and boson-boson interaction potentials the energy and density per particle are exactly reproduced by the mean field in the infinite-particle limit, independently of the dimension of the problem. In spite of this, the full wave function is rather complex and found to usually be very different from the mean-field wave function in this limit; sometimes there is even vanishing similarity between the two. This important result is explained by the correlation between the few particles in the depleted manifold with the very many particles in the condensed manifold. New physical insight is also obtained for two explicit examples in the infinite-particle limit, one with long- and one with short-range interactions. In particular, the phonon Hamiltonian could be solved in closed form in both cases and the wave functions are discussed. For the first example the wave function is provided in closed form and the impact of the center of mass on the wave function is explicitly demonstrated.

Enlarging the trap leads to an increase of the depletion. This trend is already reflected in second order of the perturbation theory (see also the exact results for the applications presented in Secs. IV and V in the infinite-particle limit). It is interesting to contrast here the homogeneous and inhomogeneous cases as $N \to \infty$. In the homogeneous case the depletion is a fraction, say f. Even if this fraction is small, it scales with N and the number of bosons in the depleted fraction is fN, i.e., infinite in the thermodynamic limit. In the trap the depletion of the inhomogeneous system is a constant for a given trap and interaction strength; i.e., the number of bosons in the depleted manifold is finite and hence vanishes when divided by N. One cannot transfer the results obtained for inhomogeneous systems to the thermodynamic limit. The present theory is applicable as long as the trap size is finite.

Finally, we would like to touch upon two issues. First, the phonon Hamiltonian has been derived for infinitely many bosons. We stress, however, that the results obtained with the phonon Hamiltonian also apply for finite numbers of bosons. For weak interaction strength this has been explicitly shown by the perturbation expansion, where the leading term for all quantities (also for the wave function) studied depends on the particle number only via the factor $\frac{N}{N-1}$. If the interaction strength becomes stronger, the dependence on N is still weak once N is sufficiently large. What exactly "sufficiently large" means depends for a given value of Λ on the trap and interaction potentials employed. The numerical results in [12] show that already with $N = 10^5$ one can achieve converged calculations for the overlap, which are numerically the same as for $N = 10^7$.

Second, although the present work is on stationary states of the interacting boson system, the results can also be used in many cases to describe dynamics. The dynamics of a system can often be expressed by a superposition of ground and excited states. As the present theory also allows one to compute excited states and their energy, at least in the infinite-particle limit, one can have access to dynamics. Alternatively, one can use the phonon Hamiltonian directly to describe the dynamics. All of this is, however, only possible as long as the dynamics is not so fierce as to destroy the basis for the derivation of the phonon Hamiltonian, namely that the system stays essentially condensed.

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