Coupled-cluster theory for systems of bosons in external traps

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A coupled-cluster approach for systems of N bosons in external traps is developed. In the coupled-cluster approach the exact many-body wave function is obtained by applying an exponential operator $\exp\{T\}$ to the ground configuration $|\phi_0\rangle$. The natural ground configuration for bosons is, of course, when all reside in a single orbital. Because of this simple structure of $|\phi_0\rangle$, the appearance of excitation operators $T=\Sigma_{n=1}^{N}T_n$ for bosons is much simpler than for fermions. We can treat very large numbers of bosons with coupled-cluster expansions. In a substantial part of this work, we address the issue of size consistency for bosons and enquire whether truncated coupled-cluster expansions are size consistent. We show that, in contrast to the familiar situation for fermions for which coupled-cluster expansions are size consistent, for bosons the answer to this question *depends* on the choice of ground configuration. Utilizing the natural ground configuration, working equations for the truncated coupled-cluster with $T=T_1+T_2$, i.e., coupled-cluster singles doubles are explicitly derived. Finally, an illustrative numerical example for a condensate with up to $N=10\,000$ bosons in an harmonic trap is provided and analyzed. The results are highly promising.

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I. INTRODUCTION

Following the experimental demonstrations of Bose-Einstein condensates in dilute gases [1,2], the problem of many bosonic atoms interacting in a trap potential has attracted an accelerated interest by the scientific community, see Refs. [3,4], and references therein. There are many phenomena trapped bosons exhibit that can be described quite well by the standard mean-field approach, namely, Gross-Pitaevskii (GP) theory [5], see Refs. [3,4], and reference therein. Side-by-side, the necessity to go beyond mean-field and describe many-body facets of trapped bosons has become well accepted and pursued by the community, see the reviews [6,7], and references therein.

The many-boson problem is difficult to tackle. Consider, for instance, the standard configuration-interaction (CI) approach which employs a basis set expansion. When the interaction between the N bosons is substantial and/or many of them are present, the number of configurations necessary to properly describe the correlated wave function quickly increases beyond computational reach and truncations become a must. When truncations of the CI expansion are made, there are hints and evidences to slow convergence of the CI expansion, see, e.g., Refs. [8,9]. Evidently, development of other many-body methods which truncate the full configuration space in a different manner are of high relevance and actuality. Such methods are reviewed in Refs. [6,7], the latter being devoted to the extensively studied homogeneous Bose gas problem.

Coupled-cluster theory was first formulated in nuclear physics by Coester [10] and Coester and Kümmel [11], and soon after was introduced to electron-structure theory by Čižek [12] and Čižek and Paldus [13]. Coupled-cluster theory has since proven to be a very valuable and accurate approach in the many-fermion problem, see Refs. [14–16], and references therein. For atomic and molecular systems, coupled-cluster theory is currently considered to be one of the, if not the, most powerful many-body tool for calculating electron-correlation energies [14–16], also in relativistic systems [17]. In the coupled-cluster approach the exact many-body wave function is obtained by applying an exponential operator $\exp\{T\}$ to the ground configuration $|\phi_0\rangle$. In practice, one truncates of course the operator T. For fermions, it is widely known that truncated coupled-cluster expansions are size consistent, which is another advantage the coupled-cluster approach possesses in comparison to truncated CI expansions which are not size consistent [18].

Our aim in this work is to derive a coupled-cluster theory for bosons with emphasis on systems of interacting indistinguishable bosons in traps with up to many particles. We investigate aspects such as size consistency and what to use as the initial ground configuration $|\phi_0\rangle$. We would like to mention that coupled-cluster approaches for molecular vibrations [19], "bosonic nuclei" [20], the spin-boson model [21], and within bosonization of many-electron systems [22] have been studied in the literature, but are very different from the present work.

The structure of the paper is as follows. In Sec. II, we briefly discuss the standard configuration-interaction approach. In Sec. III, the coupled-cluster theory for bosons is developed, where the issue of size consistency is extensively analyzed. Working equations for a truncation of the coupled-cluster to single and double excitations (CCSD) are derived in Sec. IV, and an illustrative numerical example is provided in Sec. V. Finally, summary and conclusions are drawn in Sec. VI.

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II. THE STRAIGHTFORWARD APPROACH: CONFIGURATION INTERACTION

Consider a system of interacting N identical particles, for simplicity either spinless or all of the same spin projection. We introduce M one-particle functions $\varphi_i(\vec{r}), i=1,2,\ldots,M$, which are called orbitals. The N particles can be distributed over these orbitals and each allowed distribution defines a configuration $\Phi_{i_1,i_2,\ldots,i_N}$. If the particles are fermions, the configuration is a determinant

$$\Phi_{i_1,i_2,\ldots,i_N} = \hat{\mathcal{A}}\varphi_{i_1}\varphi_{i_2}\ldots\varphi_{i_N} \tag{1}$$

and if they are bosons, it is a permanent

$$\Phi_{i_1,i_2,\ldots,i_N} = \hat{\mathcal{S}}\varphi_{i_1}\varphi_{i_2}\ldots\varphi_{i_N}. \tag{2}$$

$\hat{\mathcal{A}}$ and $\hat{\mathcal{S}}$ denote the antisymmetrizing and symmetrizing operators, respectively. In the absence of interaction, each configuration is an eigenfunction of the Hamiltonian H of the system. In the presence of interaction between the particles, the exact eigenfunction Ψ in the space defined by the M orbitals is given by a superposition of all the allowed configurations

$$\Psi = \sum_{i_1,i_2,\ldots,i_N} D_{i_1,i_2,\ldots,i_N}\Phi_{i_1,i_2,\ldots,i_N}, \tag{3}$$

where the D's are complex numbers. The D's are usually determined variationally by diagonalizing the Hamiltonian matrix $\{\langle\Phi_{i_1,i_2,\ldots,i_N}|H|\Phi_{j_1,j_2,\ldots,j_N}\rangle\}$. Clearly, to obtain the correct exact eigenfunction, the orbital basis should be complete, i.e., $M\to\infty$, but in practical calculations M is kept finite.

How many distinct configurations participate in the CI expansion (3)? Two fermions cannot reside in a single orbital and, therefore, the number of configurations is simply given by

$$\mathcal{F}_N^M = \binom{M}{N}. \tag{4}$$

In the case of bosons there is no restriction on how many particles can reside in an orbital. We find that the number of bosonic configuration reads

$$\mathcal{B}_N^M = \binom{M+N-1}{N}. \tag{5}$$

These numbers grow rapidly with the size M of the orbital basis and much more rapidly for bosons than for fermions. Consider, for example, 165 particles. For fermions $M=165$ is needed in order to have a single configuration. Adding just five more orbitals, i.e., $M=170$, increases the number of configurations to over a billion (10^9). For bosons, $M=1$ is needed to have a single configuration and employing $M=170$ leads to an astronomically large number of configurations.

For 165 fermions to have only five additional (so-called virtual) orbitals at their disposal is usually insufficient for the calculation of their correlation energy. For an accurate calculation more virtual orbitals are required making the straightforward CI approach impractical. Fortunately, the number of orbitals needed for accurate calculations for bosons is much less than for fermions. Because many or even all bosons may reside in a single orbital, the structure of the orbitals used play a major role in the calculation and the appropriate choice of the orbitals is essential. The orbitals are preferentially determined self-consistently as done, for instance, by the use of the GP equation [5], see also Refs. [3,4]. Nevertheless, to achieve meaningful results M is not small and the number of configurations is often beyond reach. To return to our example of $N=165$, the number of configurations exceeds a billion with just $M=6$, i.e., with just five additional (virtual) orbitals. Note that the numbers of bosonic and fermionic configurations are identical for the same number of virtual orbitals ($M-N$ orbitals for fermions and $M-1$ for bosons) as can be seen from Eqs. (4) and (5).

In the following we concentrate on bosons and make use of the destruction and creation operators b_i and $b_i^\dagger$, $i=1,2,\ldots,M$, corresponding to the orbitals φ_i introduced above. These operators fulfill the usual commutator relations

$$[b_i,b_j^\dagger] = \delta_{i,j},\ [b_i,b_j] = [b_i^\dagger,b_j^\dagger] = 0 \tag{6}$$

for bosons. Utilizing these operators, we define the ground configuration

$$|\phi_0\rangle = \frac{1}{\sqrt{N!}}(b_1^\dagger)^N|0\rangle,\ \langle\phi_0|\phi_0\rangle = 1 \tag{7}$$

which is the ground state of the system in the absence of interaction between the particles. $|0\rangle$ denotes the vacuum. All other configurations $|\Phi_{i_1,i_2,\ldots,i_N}\rangle$ are obtained directly by applying excitation operators to $|0\rangle$. Singly excited configurations read $b_i^\dagger b_1|\phi_0\rangle$, doubly excited ones are given by $b_i^\dagger b_j^\dagger (b_1)^2|\phi_0\rangle$, and so on. In analogy to Eq. (3) the exact state $|\Psi\rangle$ can be expanded in these orthogonal configurations

$$|\Psi\rangle = |\phi_0\rangle + \sum_{i_1=2}^{M} d_{i_1}b_{i_1}^\dagger b_1|\phi_0\rangle + \sum_{i_1,i_2=2}^{M} d_{i_1i_2}b_{i_1}^\dagger b_{i_2}^\dagger (b_1)^2|\phi_0\rangle + \cdots + \sum_{i_1,i_2,\ldots,i_N=2}^{M} d_{i_1,i_2,\ldots,i_N}b_{i_1}^\dagger b_{i_2}^\dagger\cdots b_{i_N}^\dagger (b_1)^N|\phi_0\rangle. \tag{8}$$

For later use we choose explicitly intermediate normalization of the exact state, i.e., $\langle\phi_0|\Psi\rangle=1$, do not impose normalization on the orthogonal configurations except on $|\phi_0\rangle$, and allow for redundancy in that the same configuration may appear several times in the expansion. We note that the expansion coefficients are independent of the order of the indices: $d_{i_1,\ldots,i,\ldots,j,\ldots,i_N} = d_{i_1,\ldots,j,\ldots,i,\ldots,i_N}$. Obviously, there is a one to one correspondence between the coefficients in Eq. (8) and those in the expansion in distinct normalized configurations.

With the aid of the expansion (8) it is relatively straightforward to express the exact energy E_0 in terms of the expansion coefficients. Starting from the Schrödinger equation $H|\Psi\rangle = E_0|\Psi\rangle$ one immediately arrives at

$$E_0 = \langle \phi_0 | H | \Psi \rangle. \tag{9}$$

As usual the system's Hamiltonian consists of an one-particle operator $\hat{h}(\vec{r})$ and a two-particle interaction $\hat{V}(\vec{r}-\vec{r}')$. Expressed in destruction and creation operators H takes on the common appearance [23]

$$H = \sum h_{ij} b_i^\dagger b_j + \frac{1}{2} \sum V_{ijkl} b_i^\dagger b_j^\dagger b_k b_l, \tag{10}$$

where

$$h_{ij} = \int \varphi_i^* \hat{h} \varphi_j d\vec{r},$$

$$V_{ijkl} = \int \int \varphi_i^*(\vec{r}) \varphi_j^*(\vec{r}') \hat{V}(\vec{r}-\vec{r}') \varphi_k(\vec{r}) \varphi_l(\vec{r}') d\vec{r} d\vec{r}'. \tag{11}$$

Inserting Eqs. (8) and (10) into Eq. (9) leads to

$$[E_0 - \langle \phi_0 | H | \phi_0 \rangle]/N = \sum_{l=2}^{M} [h_{1l} + (N-1) V_{111l}] d_l + (N-1) \sum_{k,l=2}^{M} V_{11kl} d_{kl}. \tag{12}$$

The energy correction per particle due to the dressing $\phi_0 \to \Psi$ can be expressed by the coefficients $\{d_l\}$ and $\{d_{lk}\}$. The orbitals $\{\varphi_l\}$ can be conveniently chosen to simplify Eq. (12) further by eliminating the $\{d_l\}$; see next section for details.

We should keep in mind that in spite of the compactness of expression (12) this equation cannot be used to determine the unknown coefficients $\{d_l, d_{kl}\}$ since $\langle \phi_0 | H | \Psi \rangle$ in Eq. (9) is not subject to a variational principle. These coefficients are determined by diagonalizing the Hamiltonian matrix which is—as discussed above—of immense dimensionality and, in general, not amenable to practical calculations. One, therefore, resorts to approximations such as keeping M very small and/or truncating the CI expansion (8). A particularly appealing approach is to truncate the expansion by taking into account only a few classes of configurations. In analogy to electron structure calculations we may consider $|\phi_0\rangle$ and all singly excited configurations (CIS), add to these all doubly excited configurations (CISD), and so on.

III. COUPLED-CLUSTER THEORY FOR BOSONS

A. General aspects

The CI approach discussed in the preceding section is formally straightforward but impractical. Truncating the CI expansion cannot be expected to solve the problem satisfactorily in many cases. In particular, when the interaction between the bosons is substantial and/or many bosons are present, numerous highly excited configurations may contribute rendering systematic truncations impossible. We are, therefore, searching for more efficient approaches which are amenable to systematic approximations.

In the coupled-cluster approach the exact wave function is obtained by applying an exponential operator to the ground configuration (7)

$$|\Psi\rangle = e^T |\phi_0\rangle. \tag{13}$$

The operator T is a superposition of excitation operators

$$T = \sum_{n=1}^{N} T_n, \tag{14}$$

where for bosons we may write

$$T_n = t_n (b_1)^n,$$

$$t_n = \sum_{i_1,\ldots,i_n=2}^{M} c_{i_1,i_2,\ldots,i_n} b_{i_1}^\dagger b_{i_2}^\dagger \cdots b_{i_n}^\dagger. \tag{15}$$

For simplicity we have again introduced redundancies to avoid unpleasant restrictions on the summation indices. The yet unknown coefficients $c_{i_1,i_2,\ldots,i_N}$ do not depend on the ordering of the subscripts, i.e., $c_{i_1 i_2} = c_{i_2 i_1}$, etc. It is convenient to note that $[T_n, T_m] = 0$ and hence $\exp(T) = \exp(T_N) \cdots \exp(T_1)$. Because of the simple structure of $|\phi_0\rangle$, see Eq. (7), the appearance of the coupled-cluster operator T for bosons is much simpler than that for fermions, see, e.g., Refs. [12,14].

Using Eq. (13) and the Schrödinger equation it is easily seen that the exact energy reads

$$E_0 = \langle \phi_0 | e^{-T} H e^T | \phi_0 \rangle. \tag{16}$$

The wave function (13) is subject to intermediate normalization $\langle \phi_0 | \Psi \rangle = 1$ as can be deduced directly from $\langle \phi_0 | \exp(\pm T) = \langle \phi_0 |$. In this respect the situation is similar to that discussed in the preceding section, see Eq. (9). On the other hand, Eq. (16) is much more powerful because $\exp(-T) H \exp(T)$ can be evaluated using the useful expansion

$$\dot{A} \equiv e^{-T} A e^T = A + \frac{1}{1!}[A,T] + \frac{1}{2!}[[A,T],T] + \cdots, \tag{17}$$

which can be applied to any operator A.

As discussed in the preceding section, an expression similar to (16) is not subject to a variational principle and cannot be used to determine the unknown coefficients $c_{i_1,i_2,\ldots,i_n}$. To proceed we notice that $e^{-T} H e^T | \phi_0 \rangle = E_0 | \phi_0 \rangle$ and hence projecting on any excited configuration provides an equation for the coefficients. The singly excited configurations lead to the $(M-1)$ equations

$$\langle \phi_0 | b_1^\dagger b_i e^{-T} H e^T | \phi_0 \rangle = 0, \; i = 2,3, \ldots, M \tag{18}$$

and the doubly excited ones to the $M(M-1)/2$ distinct equations

$$\langle \phi_0 | (b_1^\dagger)^2 b_i b_j e^{-T} H e^T | \phi_0 \rangle = 0, \; i \geqslant j = 2,3, \ldots, M, \tag{19}$$

and so on. The number of independent equations corresponds exactly to the number of distinct coefficients, $M-1$ coefficients c_i, $M(M-1)/2$ coefficients c_{ij}, etc. The equations above are nonlinear in the unknown coefficients and, further-

more, are coupled to each other. The set (18) contains the c_i as well as the c_{ij}, while the set (19) also the c_{ijl}. Since the highest possible excitation is N-fold, the final set of equations does not contain new unknown coefficients.

The total number of distinct coefficients in Eq. (15) is, of course, identical to the total number of distinct bosonic configurations given in Eq. (5). We have argued above that this number is enormous. Moreover, equations such as Eq. (18) used to determine the coefficients are nonlinear. So where is the gain with respect to the straightforward CI method discussed in the preceding section? The gain is in the favorable properties of the coupled-cluster ansatz (13) when truncating the sum of excitation operators in Eq. (14). Let us for demonstration include only single and double excitation operators in T, i.e., $T=T_1+T_2$. Then, the only coefficients available are the c_i and c_{ij} which can be determined from Eqs. (18) and (19). By inspecting that

$$|\Psi\rangle = |\phi_0\rangle + (T_1+T_2)|\phi_0\rangle + \frac{1}{2!}(T_1^2+2T_1T_2+T_2^2)|\phi_0\rangle + \cdots \tag{20}$$

one readily notices that this expansion of the wave function contains *all possible* distinct configurations of the system. Equations (18) and (19) determine the c_i and c_{ij} coefficients such that the expansion (20) is optimal in providing $e^{-T}He^{T}|\phi_0\rangle$. In contrast to this CCSD approach as we would call it in analogy, the CISD expansion, on the other hand, knows only singly and doubly excited configurations, i.e., is rather related to truncating Eq. (20) as $|\Psi\rangle = |\phi_0\rangle + \left(T_1+\frac{1}{2!}T_1^2+T_2\right)|\phi_0\rangle$. For additional advantages of the coupled-cluster ansatz see the following two sections.

B. Impact of the single excitation operator T_1

The influence of T_1 is particularly transparent. For this purpose we consider $\exp(T_1)|\phi_0\rangle$ and remind that the ground configuration is particularly simple for bosons, see Eq. (7). Using the series (17), it is easily seen that

$$e^{T_1}b_1^\dagger e^{-T_1} = b_1^\dagger + \sum_{l=2}^{M} c_l b_l^\dagger \tag{21}$$

which defines a new creation operator

$$\tilde{b}_1^\dagger = \frac{1}{\sqrt{1+|c|^2}}\left(b_1^\dagger + \sum_{l=2}^{M} c_l b_l^\dagger\right), \tag{22}$$

where $|c|^2=\Sigma_{l=2}^{M}|c_l|^2$, which fulfills the boson commutator relation $[\tilde{b}_1,\tilde{b}_1^\dagger]=1$. Consequently, the action of $\exp(T_1)$ on the ground permanent ϕ_0 is to define a new permanent

$$|\tilde{\phi}_0\rangle \equiv e^{T_1}|\phi_0\rangle \propto (\tilde{b}_1^\dagger)^N|0\rangle \tag{23}$$

which is, however, not normalized to 1, but rather to $\langle\tilde{\phi}_0|\tilde{\phi}_0\rangle=[1+|c|^2]^N$.

To proceed, one can consider the quantities appearing in Eq. (22) as the first column of an unitary matrix $\mathbf{U}$ which defines a new set of M creation operators $(\tilde{b}_1^\dagger,\tilde{b}_2^\dagger,\ldots,\tilde{b}_M^\dagger)=(b_1^\dagger,b_2^\dagger,\ldots,b_M^\dagger)\mathbf{U}$. This transformation defines a new set of corresponding orthonormal orbitals $\tilde{\varphi}_1,\tilde{\varphi}_2,\ldots,\tilde{\varphi}_M$. In turn, the new set of creation and destruction operators or, equivalently, of orbitals, can be formally utilized to eliminate T_1 from T. The remaining operators of T, the T_n with $n\geqslant 2$, are now defined with the operators $\tilde{b}_1$ and $\tilde{b}_i^\dagger$, e.g., $T_2=\Sigma_{i_1,i_2=2}^{M}\tilde{c}_{i_1i_2}\tilde{b}_{i_1}^\dagger\tilde{b}_{i_2}^\dagger(\tilde{b}_1)^2$.

Clearly, the impact of T_1 is to introduce a new orbital $\tilde{\varphi}_1$ optimal for the coupled-cluster expansion. In particular, if we put all $T_n=0$, $n\geqslant 2$, this new orbital can be constructed explicitly. As discussed in Sec. IV, this orbital then minimizes the energy functional $\langle\phi_0|H|\phi_0\rangle$.

C. Size consistency

Let us consider a super system consisting of R noninteracting replica of our original N-particle system. Clearly, the exact energy of this super system is $E_0(R)=RE_0$, where E_0 is the energy of the N-particle system. This result will, of course, be reproduced if either the full configuration interaction expansion (8) or the coupled-cluster expansion (13)–(15) is used. In general, the full expansion cannot be utilized and one has to resort to approximations. We, therefore, have to pose the question whether truncated CI and coupled-cluster expansions for bosonic systems lead to energies which scale correctly with the number of replica R, i.e., whether these truncated expansions are size consistent.

Size consistency plays an important role in electronic structure calculations [18]. Imagine, for instance, a molecule which is being broken up into fragments or a cluster consisting of weakly interacting atoms. The computational methods used must be size consistent in order to describe correctly the break up of the molecule into fragments or the cluster. Indeed, it is well known that truncated CI expansions are generally *not* size consistent whereas truncated CC expansions are size consistent for electrons. In the following we would like to address the issue of size consistency for bosons. The concept of size consistency is also relevant for bosons. Bosonic systems, e.g., in an external double-well trap can be fragmented [24,25], and the computational method used must be able to describe fragmentation correctly. Another, even more extreme example is the superfluid to Mott-insulator transition of Bose-Einstein condensates in a lattice trap [26,27]. In the superfluid phase all bosons communicate with each other and in the insulator phase each potential well of the lattice contains a single boson which hardly interacts with the other bosons.

The ground configuration ϕ_0 of the super system is a symmetrized product of the R ground configurations of the individual replica. We write

$$|\phi_0\rangle = \frac{1}{(N!)^{R/2}}\prod_{k=1}^{R}(b_{1_k}^\dagger)^N|0\rangle, \tag{24}$$

where $b_{1_k}^\dagger$ is the creation operator for bosons in the occupied orbital of the kth replica. The Hamiltonian of the super system is, of course, just the sum of the individual Hamiltonians

$$H = H_1 + H_2 + \cdots + H_R. \tag{25}$$

We first show that the truncated CI expansion is not size consistent. For this purpose we proceed in analogy to the considerations done for fermions (electrons) [18] and assume each of the R replica to consist of two orbitals, or equivalently two destruction operators b_{1_k} and b_{2_k}, of different spatial symmetry. It is sufficient to demonstrate that CID is not size consistent. This implies that the expansion of the total wave function $|\Psi\rangle$ consists of the superposition of the ground configuration $|\phi_0\rangle$ given above in Eq. (24) and of the doubly excited configurations $(b_{2_k}^\dagger)^2(b_{1_k})^2|\phi_0\rangle$, $k=1,2,\ldots,R$. In this space the Hamiltonian matrix $\mathcal{H}$ representation of H is an "arrow" matrix of dimension $R+1$, the elements of which read

$$\mathcal{H}_{00}=\langle\phi_0|H|\phi_0\rangle,$$

$$\mathcal{H}_{0k}=C\langle\phi_0|\,H_k|(b_{2_k}^\dagger)^2(b_{1_k})^2|\phi_0\rangle,$$

$$\mathcal{H}_{kk'}=|C|^2\langle\phi_0|(b_{1_k}^\dagger)^2(b_{2_k})^2|H_k|(b_{2_k}^\dagger)^2(b_{1_k})^2|\phi_0\rangle\delta_{kk'}, \quad (26)$$

where C is the normalization constant of a double excited configuration. Note that all matrix elements $\mathcal{H}_{0k}, k=1,2,\ldots,R$ are identical to each other and so are all the $\mathcal{H}_{kk}$. We put for convenience $\mathcal{H}_{0k}=V$ and $\mathcal{H}_{kk}=\langle\phi_0|H|\phi_0\rangle+\Delta$. The diagonalization of $\mathcal{H}$ can be performed analytically by searching for the roots of $E-\langle\phi_0|H|\phi_0\rangle=\Sigma_k|\mathcal{H}_{0k}|^2/[E-\mathcal{H}_{kk}]$. This immediately leads to

$$E_0(R)=\langle\phi_0|H|\phi_0\rangle+\frac{\Delta}{2}-R^{1/2}\left[V^2+\frac{\Delta^2}{4R}\right]^{1/2} \quad (27)$$

which implies that the truncated CI expansion is not size consistent. Using Eqs. (24) and (25) one sees that the expectation value $\langle\phi_0|H|\phi_0\rangle$ is size consistent and the correction term $E_0-\langle\phi_0|H|\phi_0\rangle$ scales as $R^{1/2}$ for large R instead of being proportional to R.

In contrast to the truncated CI expansion, the truncated coupled-cluster expansion is size consistent. The operator T is a sum of $T^{(k)}$ for the $k=1,2,\ldots,R$ replica. Each of the $T^{(k)}$ has the appearance as in Eqs. (14) and (15) for the individual replica. One has just to index the destruction and annihilation operators appearing there by a further subscript k for the kth replica. The values of the coefficients c in Eq. (15) are, of course, the same for all replica. Clearly, the various $T^{(k)}$ commute with each other and, consequently, $\exp\{T\}$ can be factorized as $\Pi_{k=1}^R\exp\{T^{(k)}\}$ leading to

$$|\Psi\rangle=[e^{T^{(1)}}(b_{1_1}^\dagger)^N][e^{T^{(2)}}(b_{1_2}^\dagger)^N]\cdots[e^{T^{(R)}}(b_{1_R}^\dagger)^N]|0\rangle \quad (28)$$

which is size consistent for any truncation of the $T^{(k)}$.

In spite of the favorable structure (28) a major problem arises. If we *a priori* know that our system consists of R noninteracting replica, we may, of course, use the ϕ_0 in Eq. (24) and obtain a size consistent result. However, the intension is to apply the coupled-cluster method not knowing *a priori* how our system behaves, i.e., whether it is superfluid or breaks up into weakly interacting subsystems. Lacking this knowledge, we cannot use the ansatz (24) for ϕ_0. Resorting to

$$|\phi_0\rangle=\frac{1}{\sqrt{(NR)!}}(b_1^\dagger)^{NR}|0\rangle \quad (29)$$

which does not distinguish between the R replica as is the case in Eq. (24), we may again pose the question: is a truncated coupled-cluster ansatz size consistent?

To proceed, we first have to identify the $b_1^\dagger$ operator appearing in Eq. (29) in terms of the operators $b_{1_k}^\dagger$ of the individual replica. Since all replica are identical, we can construct R new operators $B_{11}^\dagger, B_{12}^\dagger, \ldots, B_{1R}^\dagger$ of the super system by linearly combining the $b_{1_k}^\dagger$. Without loss of generality we can always chose

$$b_1^\dagger\equiv B_{11}^\dagger=R^{-1/2}(b_{1_1}^\dagger+b_{1_2}^\dagger+\cdots+b_{1_R}^\dagger), \quad (30)$$

i.e., as a trivial superposition of the creation operators corresponding to the occupied orbitals of the individual replica. All the $B_{1i}^\dagger$ will posses different permutational symmetries which simplifies the evaluation considerably. For instance, for $R=2$ we have $B_{11}^\dagger=2^{-1/2}(b_{1_1}^\dagger+b_{1_2}^\dagger)$ and $B_{12}^\dagger=2^{-1/2}(b_{1_1}^\dagger-b_{1_2}^\dagger)$. We note that for each set of virtual orbitals an analogous procedure can be applied to introduce the remaining orbitals of the super system: $b_{2_1}^\dagger, b_{2_2}^\dagger, \ldots, b_{2_R}^\dagger$ are linearly combined to give $B_{21}^\dagger, B_{22}^\dagger, \ldots, B_{2R}^\dagger$ and so on. This results in RM creation operators of the super system emerging from the M operators of each of the replica. Since only one orbital is occupied in the ground configuration of the super systems, all the other ones are virtual orbitals, i.e., also the $B_{12}^\dagger, B_{13}^\dagger, \ldots, B_{1R}^\dagger$ refer now to virtual orbitals.

The Hamiltonian (25) and the coupled-cluster operator T are now expressed in the $B_{ik}^\dagger$ of the super system. Let us consider as an example the one-body part of H in the occupied space of the individual replica:

$$\sum_k^R h_{11}b_{1_k}^\dagger b_{1_k}=\sum_k^R h_{11}B_{1k}^\dagger B_{1k}.$$

Note that in the two-body part of the H operator products such as $B_{1k}^\dagger B_{1k'}^\dagger B_{1k}B_{1k'}, k\neq k'$, appear. Let us begin the analysis by inspecting the mean-field energy $\langle\phi_0|H|\phi_0\rangle$. Here, only the terms of the Hamiltonian containing $B_{11}^\dagger B_{11}$ and $B_{11}^\dagger B_{11}^\dagger B_{11}B_{11}$ contribute. These terms take on the explicit appearance

$$h_{11}B_{11}^\dagger B_{11}+\frac{V_{1111}}{2R}B_{11}^\dagger B_{11}^\dagger B_{11}B_{11},$$

where h_{11} and V_{1111} are the quantities defined in Eq. (11) for an individual replica. One immediately finds

$$\begin{aligned}\langle\phi_0|H|\phi_0\rangle&=NRh_{11}+\frac{NR(NR-1)}{2R}V_{1111}\\&=R\left\{Nh_{11}+\frac{N(N-1/R)}{2}V_{1111}\right\}\end{aligned} \quad (31)$$

implying that even the mean-field energy is not size consistent; a surprising result. The mean-field energy of an individual replica is $Nh_{11}+[N(N-1)/2]V_{1111}$. Consequently, size

consistency is achieved only if each individual replica contains many bosons, i.e., for $N \gg 1$.

To better understand the implications of the above finding, let us briefly consider the coupled-cluster operator T of the super system. Since now there is only a single occupied orbital (related to B_{11}), *all* the other operators $B_{ik}^{\dagger}$ relate to virtual orbitals of the super system. Consequently, T can be broken up into a part T' which contains excitations solely within the original occupied orbitals of the different replica and the remaining part T'' where excitations to the originally virtual orbitals of these replica are included. As an example we consider the double excitation operator T_2 [see Eqs. (14) and (15)]:

$$T_2 = T_2' + T_2'' = \sum_{k=2}^{R} c_k (B_{1k}^{\dagger})^2 (B_{11})^2 + \sum_{k=1}^{R} \sum_{i,j}^{M\,\prime} c_{ijk} B_{ik}^{\dagger} B_{jk}^{\dagger} (B_{11})^2. \tag{32}$$

In T_2'' the terms with B_{11} and those of T_2' are not included as indicated by the primed summation symbol Σ'. In the example of two replica, we have the T_2' excitation operator $(b_{1_1}^{\dagger} - b_{1_2}^{\dagger})^2 (b_{1_1} + b_{1_2})^2$ which is actually an excitation within the occupied manifold of the replica. Obviously T' and T'' commute.

Interestingly, the full impact of $\exp\{T'\}$ is needed in order to restore the size consistency. Indeed, a calculation shows that

$$\langle \phi_0 | e^{-T'} H e^{T'} | \phi_0 \rangle = R \left\{ N h_{11} + \frac{N(N-1)}{2} V_{1111} \right\} \tag{33}$$

which is the expected correct mean-field result and is identical to the expectation value of H obtained with the ansatz (24) for ϕ_0 where the knowledge of having R replica has been used.

The result (33) follows only if the expansion of $\exp\{T'\}$ is fully considered and not truncated. The impact of $\exp\{T'\}$ is to transform ϕ_0 in Eq. (29) into the form of Eq. (24) which is appropriate for R replica. In other words, truncated coupled-cluster expansions are not size consistent once the ansatz (29) is used for ϕ_0. The good news is that the violation of the size consistency at least for the mean-field energy leads to negligible errors for large individual systems ($N \gg 1$), see Eq. (31). In this respect bosons and fermions behave differently. Due to the fact that each fermion resides in its own orbital, size consistency in truncated coupled-cluster expansions follows straightforwardly, as was also found above for bosons starting with the ϕ_0 of Eq. (24).

D. On the choice of the ground configuration ϕ_0

In contrast to fermions, the choice of the structure of the ground configuration ϕ_0 as the starting point is crucial for bosons if fragmentation or, in particular, phase transitions such as the superfluid to Mott-insulator transition are to be studied. In the absence of interaction between the bosons, the exact ground state has the appearance $\propto (b_1^{\dagger})^N |0\rangle$. It is, therefore, natural to start in the presence of interaction from an analogously structured ground configuration ϕ_0 as done in what follows Eq. (7). In the presence of interparticle interaction we have the freedom to choose the orbitals defining the destruction and annihilation operators. At least as long as this interaction is weak, it is favorable to choose the occupied orbital which minimize the energy expectation value $\langle \phi_0 | H | \phi_0 \rangle$. This readily leads to the equation

$$[\hat{h} + (N-1)\hat{J}_{11}]\varphi_1(\vec{r}) = \mu_1 \varphi_1(\vec{r}) \tag{34}$$

which determines the occupied orbital $\varphi_1(\vec{r})$. The number μ_1 can be called orbital energy or chemical potential. The direct interaction operator $\hat{J}_{11}$ is a local operator and reads

$$\hat{J}_{11} = \int \varphi_1^*(\vec{r}\,') \hat{V}(\vec{r} - \vec{r}\,') \varphi_1(\vec{r}\,') d\vec{r}\,'. \tag{35}$$

Equation (34) defines an Hermitian Fock-like operator

$$\hat{F} \equiv \hat{h} + (N-1)\hat{J}_{11},$$

$$\hat{F}\varphi_i = \mu_i \varphi_i, \tag{36}$$

the eigenfunctions of which define a complete set of orthogonal orbitals to be used in the coupled-cluster calculation.

For convenience (see Sec. IV) one may introduce the more physical operator $\hat{\tilde{F}}$

$$\hat{\tilde{F}} \equiv \hat{h} + \frac{N-1}{2}[\hat{J}_{11} + \hat{K}_{11}],$$

$$\hat{\tilde{F}}\varphi_i = \mu_i \varphi_i \tag{37}$$

which also contains the nonlocal exchange interaction operator $\hat{K}_{11}$:

$$\hat{K}_{11}\varphi_i = \int \varphi_1^*(\vec{r}\,') \hat{V}(\vec{r} - \vec{r}\,') \varphi_i(\vec{r}\,') \varphi_1(\vec{r}) d\vec{r}\,'. \tag{38}$$

Because of the structure of ϕ_0, both $\hat{F}$ and $\hat{\tilde{F}}$ produce the same occupied orbital φ_1 and the same chemical potential. All other orbitals and orbital energies are generally different. To avoid confusion, we shall indicate in the following which set of orbitals has been used. Finally, we would like to point out that if one chooses $\hat{V}(\vec{r} - \vec{r}\,') \propto \delta(\vec{r} - \vec{r}\,')$, both $\hat{F}\varphi_1 = \mu_1 \varphi_1$ and $\hat{\tilde{F}}\varphi_1 = \mu_1 \varphi_1$ reduce to the well-known and widely used GP equation [3,4].

As long as the system does not undergo a break up like in the superfluid to Mott-insulator transition in an optical lattice potential ϕ_0 of Eq. (7) and the orbital set of Eq. (36) or, preferentially, of Eq. (37) can be used in the coupled-cluster calculations. What to do when a break up is possible? Here, we would like to stress that Eq. (34) has been obtained from the minimization of the mean-field energy $\langle \phi_0 | H | \phi_0 \rangle$ within the ansatz (7) for ϕ_0. But, this ansatz does not necessarily lead to the lowest possible mean-field energy, i.e., it is not necessarily the best mean-field ansatz. The best mean-field ansatz allows the bosons to reside in different orbitals [28]:

$$|\phi_0\rangle \propto (b_r^\dagger)^{n_r}\cdots(b_2^\dagger)^{n_2}(b_1^\dagger)^{n_1}|0\rangle,\ n_1+n_2+\cdots n_r=N. \tag{39}$$

The number r of different orbitals as well as the occupation numbers $n_i, i=1,2,\ldots, r$ which tell us how many bosons reside in which orbital, are not *a priori* fixed numbers but are determined variationally to minimize the mean-field energy. The r optimal orbitals involved are, of course, also determined variationally. For brevity of presentation, we do not present the equations of the best mean-field approach and refer to the literature [28].

The best mean-field ansatz has been shown to be flexible enough to predict and describe fragmentation and superfluid and a whole zoo of insulator phases [24,25,29]. We, therefore, have reason to expect that Eq. (39) provides a useful starting point for many coupled-cluster studies. Other ways to determine the orbitals and their occupation numbers can also be anticipated in connection with the coupled-cluster approach.

IV. DERIVATION OF THE WORKING EQUATIONS

In this section the working equations of the coupled-cluster approach are derived and discussed. We concentrate here on the ansatz $\frac{1}{\sqrt{N!}}(b_1^\dagger)^N|0\rangle$ for the ground configuration for which all the necessary ingredients have been introduced and discussed in the preceding section. Working equations can also be derived starting from ansatz (39) for ϕ_0. This ground configuration contains several occupied orbitals and consequently the working equations are more elaborate.

We begin by transforming the boson destruction and creation operators with $\exp\{T\}$. Using the expansion (17) one readily finds that ($\dot{A}\equiv e^{-T}Ae^{T}$)

$$\dot{b}_1 = b_1,$$

$$\dot{b}_i^\dagger = b_i^\dagger,\ i=2,3,\ldots,M. \tag{40}$$

The destruction operator corresponding to the orbital occupied in ϕ_0, and the creation operators of the virtual orbitals are invariant to the coupled-cluster transformation. In contrast, the respective dual operators change

$$\dot{b}_1^\dagger = b_1^\dagger - \mathcal{L}_1,$$

$$\dot{b}_i = b_i + \mathcal{L}_i, \tag{41}$$

where

$$\mathcal{L}_1 = \sum_{n=1}^{N} n t_n (b_1)^{n-1},$$

$$\mathcal{L}_i = \sum_{n=1}^{N} n t_n^{(i)} (b_1)^n. \tag{42}$$

The operators t_n can be found in Eq. (15) and the operators $t_n^{(i)}$ operate in the virtual space and read

$$t_n^{(i)} = \sum_{i_2,i_3,\ldots,i_n=2}^{M} c_{i,i_2,i_3,\ldots,i_n} b_{i_2}^\dagger b_{i_3}^\dagger \cdots b_{i_n}^\dagger,$$

$$t_1^{(i)} = c_i. \tag{43}$$

In the calculations below it is gratifying to note that the $\mathcal{L}$ operators commute

$$[\mathcal{L}_i,\mathcal{L}_j] = [\mathcal{L}_1,\mathcal{L}_i] = 0 \tag{44}$$

and that their action on $\langle\phi_0|$ from the right is simple:

$$\langle\phi_0|\mathcal{L}_1 = 0,\ \langle\phi_0|(b_1)^m\mathcal{L}_1 = 0,$$

$$\langle\phi_0|\mathcal{L}_i = c_i\langle\phi_0|b_1. \tag{45}$$

To proceed, we break up the Hamiltonian (10) into several terms according to the number of operators related to the occupied orbital φ_1. The transformed one-body part $\dot{H}_0$ of the Hamiltonian then consists of four terms

$$\dot{H}_0 = h_{11}\dot{b}_1^\dagger b_1 + \sum_{k=2}^{M} h_{1k}\dot{b}_1^\dagger \dot{b}_k + \sum_{k=2}^{M} h_{k1} b_k^\dagger b_1 + \sum_{k,l=2}^{M} h_{kl} b_k^\dagger \dot{b}_l \tag{46}$$

out of which the second is the most involved one. The transformed two-body operator $\dot{V}$ contains many contributions which can be casted into nine terms which, for ease of presentation, are listed in the Appendix.

We now calculate the energy $E_0=\langle\phi_0|\dot{H}|\phi_0\rangle$, see Eq. (16). The first term of $\dot{H}_0$ in Eq. (46) and that of $\dot{V}$ in the Appendix contribute because of Eq. (45) only to the mean-field energy giving

$$\langle\phi_0|H|\phi_0\rangle = N\left[h_{11} + \frac{N-1}{2}V_{1111}\right]. \tag{47}$$

The only terms contributing to the energy correction $E_0-\langle\phi_0|H|\phi_0\rangle$ are the second term of $\dot{H}_0$ in Eq. (46) and the second and fourth terms of $\dot{V}$ in the Appendix. The final result for the exact energy reads

$$E_0 = \langle\phi_0|H|\phi_0\rangle + N\left\{\sum_{k=2}^{M}[h_{1k}+(N-1)V_{111k}]c_k + \frac{N-1}{2}\sum_{k,l=2}^{M} V_{11kl}(2c_{kl}+c_k c_l)\right\}. \tag{48}$$

Inspection of this expression makes clear from which of the

above mentioned contributing terms the various matrix elements originate. The appearance of the result (48) is similar to that derived by the straightforward configuration interaction approach, see Eq. (12). The major difference is in the $c_k c_l$ term which is missing in the CI expression (12) and arises due to the contribution of the single excitation operator T_1 to the wave function, see Eq. (20).

Until now the orbitals used are arbitrary and have not been specified. If we utilize the optimized orbitals arising from the Fock-like operators $\hat{F}$ and $\hat{\bar{F}}$ discussed in Sec. III D, we obtain in *both cases* the same result for the exact energy

$$E_0 = \langle \phi_0 | H | \phi_0 \rangle + \frac{N(N-1)}{2} \sum_{k,l=2}^{M} V_{11kl}(2c_{kl} + c_k c_l). \quad (49)$$

The other term in Eq. (48) has disappeared due to the fact that $\langle \varphi_k | \hat{F} | \varphi_1 \rangle = 0$, see Eqs. (36) and (37). In analogy to the notion of electron correlation energy [18] we might call the correction $E_0 - \langle \phi_0 | H | \phi_0 \rangle$, which is caused by the interparticle interaction beyond the mean field, boson correlation energy.

To determine the coefficients $\{c_{kl}\}$ and $\{c_k\}$ we have to evaluate the series of coupled equations (18) and (19) and so on as discussed in Sec. III A. The series consists of N sets of such equations, one set for each type of excitation operator $T_n, n=1,2,\ldots,N$. In practical calculations the expansion $T=\Sigma T_n$ is truncated. For instance, if T_1 and T_2 are considered and the $T_n, n \geqslant 3$, are put to zero, then only the sets of equations (18) and (19) must be considered in order to determine the derived coefficients. In the following we calculate this CCSD approach as we may call it.

Whereas the expression (49) for the energy is invariant to the choice of either $\hat{F}$ or $\hat{\bar{F}}$ to define the orbital basis used, the equations determining the coefficients do depend on this choice. We have computed these equations for an arbitrary set of orthonormal orbitals, but present here only the results obtained with the orbitals of $\hat{\bar{F}}$. Let us begin with $\langle \phi_0 | b_1^\dagger b_i \dot{H} | \phi_0 \rangle = 0$. From the nine terms of $\dot{V}$ shown in the Appendix it is easy to see that the fifth, eighth, and ninth terms do not contribute as they all exhibit two creation operators for virtual orbitals. All other terms contribute. Using Eqs. (41)–(45) we obtain a set of $M-1$ coupled equations $(i=2,3,\ldots,M)$

$$(\mu_1 - \mu_i)c_i = \sum_{k=2}^{M} h_{1k}(2c_{ki} + c_k c_i) + (N-1)\left\{ \frac{1}{2}\sum_{k=2}^{M} (V_{1i1k} + V_{1ik1})c_k + \sum_{k,l=2}^{M} (V_{1ikl} - V_{11kl}c_i)(2c_{kl} + c_k c_l) + (N-2)\sum_{k,l=2}^{M} V_{11kl}(3c_{kli} + c_k c_{li} + c_l c_{ki}) \right\}. \quad (50)$$

This set of equations is the result of the exact evaluation of $\langle \phi_0 | b_1^\dagger b_i \dot{H} | \phi_0 \rangle = 0$ and thus contains the coefficients c_{kli} of T_3. These coefficients have to be put equal to zero if CCSD is to be evaluated. Consulting Sec. III B we see that $c_k \neq 0$ implies the introduction of a new optimized orbital and we may assume that in CCS and $M \to \infty$ this orbital is just the eigenfunction φ_1 of $\hat{F}$ (or, equivalently, $\hat{\bar{F}}$).

To complete the CCSD we have to solve also for the set of $M(M-1)/2$ distinct coupled equations resulting from $\langle \phi_0 | (b_1^\dagger)^2 b_i b_j \dot{H} | \phi_0 \rangle = 0$, see text around Eq. (19). Here, all terms of $\dot{H}$ contribute except of the third term of $\dot{H}_0$ in Eq. (46). Using the relations (41)–(45) and the expressions of $\dot{H}$ given in Eq. (46) and in the Appendix, the derivation of the coupled equations is lengthy but straightforward. In principle, one could derive diagrammatic rules to simplify the procedure in analogy to the situation for fermions [12,13], but this is unnecessary for bosonic systems, at least as long as ϕ_0 in Eq. (7) is used. The resulting set of coupled equations reads $(i,j=2,3,\ldots,M)$

$$\begin{aligned} 2(2\mu_1 - \mu_i - \mu_j)c_{ij} - V_{ij11} - (2c_{ij} + c_i c_j)V_{1111} &= \sum_{k=2}^{M} (V_{ijk1} + V_{jik1})c_k - (V_{i111}c_j + V_{j111}c_i) \\ &+ \sum_{k=2}^{M} [(V_{1i1k} + V_{1ik1})\alpha_{kj} + (i \leftrightarrow j)] + \sum_{k=2}^{M} V_{111k}\beta_{kij} \\ &+ \sum_{k,l=2}^{M} V_{11kl}\gamma_{klij} - \sum_{k,l=2}^{M} (V_{1ikl}c_j + V_{1jkl}c_i)c_k c_l \\ &+ \sum_{k,l=2}^{M} V_{ijkl}(2c_{kl} + c_k c_l). \end{aligned} \quad (51)$$

In contrast to Eq. (50) which contains c_{kli} coefficients arising from T_3, we have concentrated in Eq. (51) on CCSD and put all coupled-cluster operators $T_n, n \geqslant 3$, to zero. The quantities α, β, and γ appearing in Eq. (51) are given by

$$\alpha_{kj} = c_{kj}(N-3) - c_k c_j,$$

$$\beta_{kij} = 2[(c_{kj}c_i + c_{ki}c_j)(3N-5) + 2c_{ij}c_k(N-2) + c_i c_j c_k],$$

$$\begin{aligned} \gamma_{klij} = {} & 4c_{ki}c_{lj}(N-2)(N-3) - 2(N-2)[2c_{ij}(2c_{kl} + c_k c_l) \\ & + c_{ki}c_l c_j + c_{li}c_k c_j + c_{kj}c_l c_i + c_{lj}c_k c_i] \\ & - (2c_{kl} + c_k c_l)(2c_{ij} - c_i c_j). \end{aligned} \quad (52)$$

It is worth noting that Eq. (50) arising from $\langle \phi_0 | b_1^\dagger b_i \dot{H} | \phi_0 \rangle = 0$ are all homogeneous, whereas Eq. (51) originating from $\langle \phi_0 | (b_1^\dagger)^2 b_i b_j \dot{H} | \phi_0 \rangle = 0$ are inhomogeneous. The inhomogeneity V_{ij11} is due to the fifth term of $\dot{V}$ given in the Appendix, i.e., from the only term which is invariant to the $\exp(T)$ transformation.

Before closing this section let us briefly discuss CCS. Here, we have to put in Eq. (50) all the $c_{kli}=0$ as well as all the $c_{kl}=0$ and disregard the set of equations (51). The resulting equations are homogeneous in the c_k coefficients and $c_k=0$ is a proper solution. This implies that CCS leads to that mean-field energy which is the minimum of $\langle \phi_0 | H | \phi_0 \rangle$, see

Sec. III D. Would we have not used the orbitals of $\hat{\hat{F}}$ but rather some set of arbitrary orthonormal orbitals, then Eq. (50) will become an inhomogeneous equation and $c_k \neq 0$.

V. ILLUSTRATIVE EXAMPLE

As an example we apply the CCSD approach to N interacting bosons in an external trap and restrict the orbital space to two real orbitals φ_1 and φ_2 of different spatial symmetry. Consequently, the CCSD (or equivalently the CCD) wave function reads $|\Psi\rangle=\exp[c_{22}(b_2^\dagger)^2(b_1)^2]|\phi_0\rangle$. In other words, the wave function depends only on a single unknown parameter c_{22}. It is easily seen that

$$|\Psi\rangle = \sum_{m=0}^{N/2} \frac{c_{22}^m}{m!}\left[\frac{N!\,(2m)!}{(N-2m)!}\right]^{1/2}|N-2m,2m\rangle, \tag{53}$$

where for simplicity we assume N to be an even number and $|m,m'\rangle$ is the normalized configuration with m bosons in φ_1 and m' bosons in φ_2.

We remind the reader that in coupled-cluster theory intermediate normalization of the wave function is used, $\langle\phi_0|\Psi\rangle=1$, and define the norm of the wave function

$$\mathcal{N}=\langle\Psi|\Psi\rangle. \tag{54}$$

Using Eq. (53) it is readily shown that this norm obeys a local "decay" law as a function of the parameter c_{22}:

$$\frac{d\mathcal{N}}{dc_{22}} = \frac{\langle n_2\rangle}{c_{22}}\mathcal{N}, \tag{55}$$

where $\langle n_2\rangle$ is the expectation value of the occupation number of bosons in orbital φ_2. Because of the different spatial symmetry of φ_1 and φ_2, these orbitals are the eigenfunctions of the reduced one-particle density matrix (natural orbitals) and the respective eigenvalues are $\langle n_1\rangle$ and $\langle n_2\rangle$ with $\langle n_1\rangle+\langle n_2\rangle=N$. Clearly,

$$\langle n_2\rangle = \langle\Psi|b_2^\dagger b_2|\Psi\rangle/\langle\Psi|\Psi\rangle, \tag{56}$$

which can be evaluated by using Eq. (53). Analogously, the variance of the occupation number of bosons in orbital φ_2 can be obtained from the second derivative of the norm

$$\frac{d^2\mathcal{N}}{dc_{22}^2} = \frac{\langle n_2^2\rangle-\langle n_2\rangle}{c_{22}^2}\mathcal{N}, \tag{57}$$

where $\langle n_2^2\rangle=\langle\Psi|(b_2^\dagger b_2)^2|\Psi\rangle/\langle\Psi|\Psi\rangle$. In the absence of interaction between the bosons, $c_{22}=0$ and $\langle n_2\rangle=0$, $\mathcal{N}=1$. As the interaction strength grows, the value of the coupled-cluster coefficient $|c_{22}|$ grows as well and with it the mean number of bosons in the orbital φ_2. The quantity $|\langle n_2\rangle/c_{22}|$ increases and determines the rate of change of the norm according to Eq. (55).

To be specific, we consider now the widely used, one-dimensional harmonic trap potential $-\frac{1}{2}\frac{\partial^2}{\partial x^2}+\frac{1}{2}x^2$, and use the contact interaction $\hat{V}(x-x')=\lambda_0\delta(x-x')$, see Refs. [3,4], and references therein. We would like to examine here the performance of the CCSD approach. It should be reemphasized that the CCSD wave function contains only a single parameter c_{22}. To solve for this parameter Eq. (51) can be used which reduces to the simple quadratic equation

$$c_{22}^2\alpha(N^2-7N+9)+c_{22}[(\mu_2-\mu_1)+\alpha(N-3)+\beta] + \alpha/4=0, \tag{58}$$

where

$$\alpha=\lambda_0\int|\varphi_1(x)|^2|\varphi_2(x)|^2dx,$$

$$\beta=\frac{\lambda_0}{2}\left(\int|\varphi_1(x)|^4dx+\int|\varphi_2(x)|^4dx\right).$$

Note that μ_1 here is the usual chemical potential of the GP equation. The ground-state energy of the CCSD approach reads

$$E_0(\mathrm{CCSD}) = E_{\mathrm{GP}} + N(N-1)\alpha c_{22}. \tag{59}$$

Here, $E_{\mathrm{GP}}=\langle\phi_0|H|\phi_0\rangle$ is the usual ground state GP energy

$$E_{\mathrm{GP}} = N\left[h_{11}+\frac{N-1}{2}\lambda_0\int|\varphi_1(x)|^4dx\right]. \tag{60}$$

For completeness we would like to compare our CCSD results with those of the CISD. The latter wave function also contains only one parameter d_{22} (see Sec. II) and the expression for the energy $E_0(\mathrm{CISD})$ is identical to that in Eq. (59) if we replace c_{22} by d_{22}. The CISD wave function is, however, a superposition of only the two configurations $|N,0\rangle$ and $|N-2,2\rangle$. The value of the parameter can be simply obtained by diagonalizing the Hamiltonian H in the space of these two configurations. This leads to the quadratic equation

$$d_{22}^2\alpha N(N-1)-2d_{22}[(\mu_2-\mu_1)+\alpha(N-3)+\beta]-\alpha/2=0 \tag{61}$$

for the configuration interaction parameter.

The results of our numerical example are summarized in Figs. 1–3. In Fig. 1 we test the performance of CCSD method in terms of the correlation energy. The correlation energy is defined as the difference between the Gross-Pitaevskii energy E_{GP} and the exact energy $E_0(\mathrm{exact})$. The latter is obtained in our model by diagonalizing the many-body Hamiltonian within the full configuration-interaction space spanned by $|m,m'\rangle, m=0,\ldots,N, m'=N-m$. We first calculate the CCSD energy $E_0(\mathrm{CCSD})$ using Eqs. (34)–(36) and (58)–(60). How much of the exact correlation energy $E_{\mathrm{GP}}-E_0(\mathrm{exact})$ is captured by CCSD is given in percent by $\%E_{\mathrm{correlation}}=100\frac{E_{\mathrm{GP}}-E_0(\mathrm{CCSD})}{E_{\mathrm{GP}}-E_0(\mathrm{exact})}$. We have calculated $\%E_{\mathrm{correlation}}$ for $N=100$, 1000, and 10 000 for several values of the interaction strength λ_0. The results are plotted in Fig. 1 versus the coupling constant $\lambda=\lambda_0(N-1)$, which is the only interaction parameter entering the GP energy, see Eq. (60). For comparison, the corresponding values obtained by the CISD method were calculated as well. We remind that both methods contain one parameter only, c_{22} and d_{22}, respectively. It is seen that the CCSD is remarkably successful in obtaining the correlation energy, with absolute error of less than 4% up to a

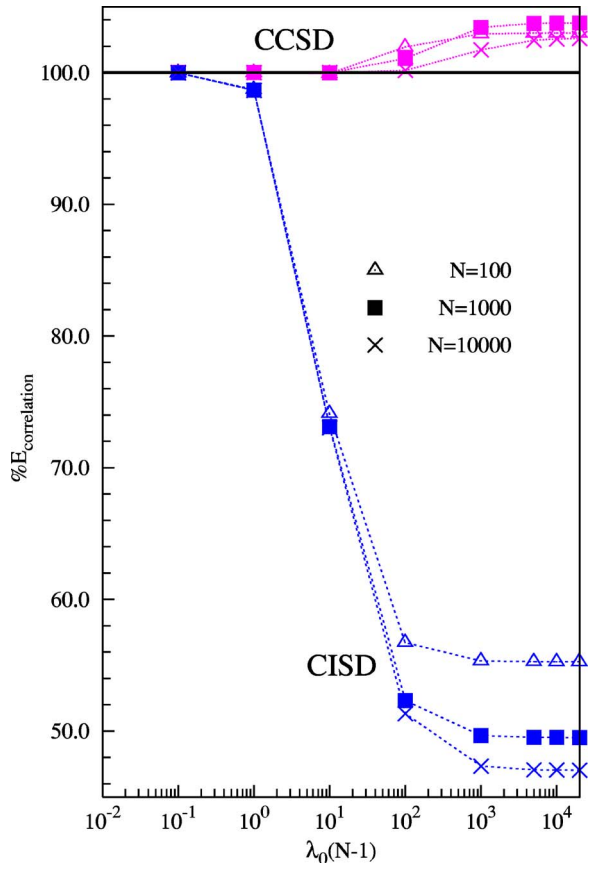

FIG. 1. (Color online) Performance of CCSD method: correlation energy. Shown is the percent of correlation energy, denoted by $\%E_{\text{correlation}}$, obtained by the CCSD for $N=100, 1000, 10\,000$ bosons and several values of interaction strength λ_0. The correlation energy is defined as the difference between the Gross-Pitaevskii energy E_{GP} and the exact energy. The exact energy is obtained in our model by diagonalizing the many-body Hamiltonian within the full configuration-interaction space. For comparison, the corresponding values obtained by CISD are also plotted.

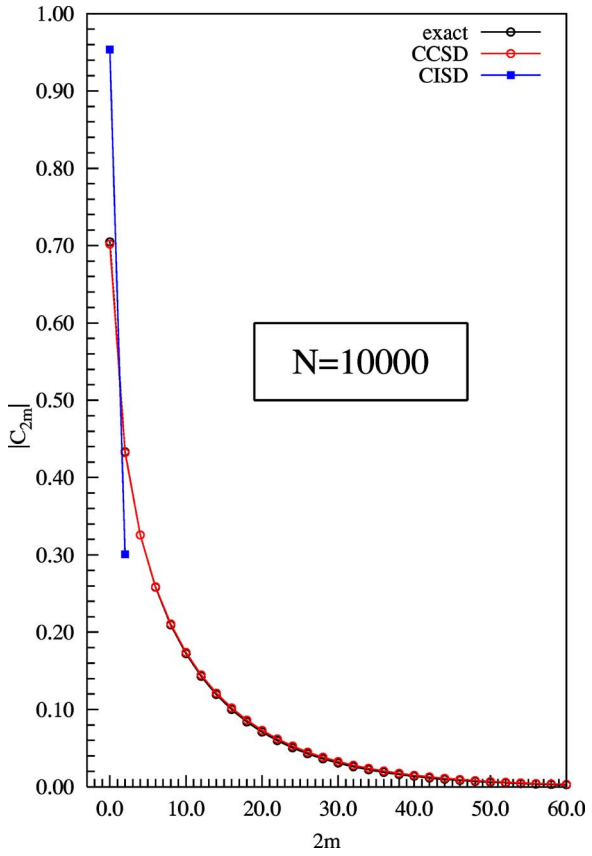

FIG. 2. (Color online) Performance of CCSD method: many-body wave function. Shown are the coefficients C_{2m} of the normalized many-body wave function $\Sigma_{m=0}^{N/2} C_{2m}|N-2m,2m\rangle$, for $N=10\,000$ bosons and $\lambda=\lambda_0(N-1)=100$ obtained by the CCSD method, see Eqs. (53) and (54). Although the coupling constant is large, it is remarkable that the CCSD C_{2m} coefficients almost perfectly match the exact coefficients, namely the red curve "sits" atop the black curve. For comparison, the two coefficients of the CISD are also shown, which deviate much from the exact solution.

huge coupling constant $\lambda=2\times10^4$. The quality of the CISD, on the other hand, starts to deteriorate already from $\lambda=1$ on and saturates at about 50%, see Fig. 1. Another result observed in Fig. 1 is that the performance of CCSD in terms of $\%E_{\text{correlation}}$ improves with increasing N, whereas that of CISD worsens.

Next, let us examine the many-body wave function obtained by the CCSD method and compare it to the exact one. For this, we first normalize the CCSD wave function (53) and express it as $\Sigma_{m=0}^{N/2} C_{2m}|N-2m,2m\rangle$. In Fig. 2 the absolute value of the C_{2m} coefficients (they alternate in sign because c_{22} is negative) for $N=10\,000$ bosons and $\lambda=100$ are plotted. Although the coupling constant is large, it is remarkable that the CCSD C_{2m} coefficients almost perfectly match the exact coefficients and it is difficult to distinguish between the red and black curves of Fig. 2. Another property of the many-body wave function when λ is growing is that the tail of the coefficients C_{2m} is extending further, showing that more and more excited configurations contribute to the many-body wave function. For comparison, the two coefficients of the CISD are also shown, which deviate much from the exact solution, see Fig. 2.

Finally, we examine the capability of the CCSD method to reproduce the exact ground-state depletion, i.e., the average number $\langle n_2\rangle$ of bosons occupying the orbital φ_2. As mentioned above, $\langle n_2\rangle$ and $\langle n_1\rangle=N-\langle n_2\rangle$ are the eigenvalues of the reduced one-body density and hence are a very sensitive tool for the quality of the CCSD many-body wave function.

We have calculated $\langle n_2\rangle$ for $N=100$, 1000, and 10 000 for several values of the interaction strength λ_0 up to the huge value of $\lambda=2\times10^4$. The results are plotted in Fig. 3 together with the exact ones and the corresponding values obtained with CISD. It is seen that the CCSD is extremely successful in obtaining the depletion $\langle n_2\rangle$ up to a large coupling constant $\lambda=10^2$. From about this value on, the quality of the CCSD wave function in terms of $\langle n_2\rangle$ depends on the specific number N of bosons. For $N=100$ it is very good for all values of λ. For $N=10\,000$ at the extreme value $\lambda=2\times10^4$ it predicts 2.5 as much depletion as the exact many-body wave function gives, namely, almost 20 bosons instead of 8 out of 10 000 bosons. We remind the reader that all these results are

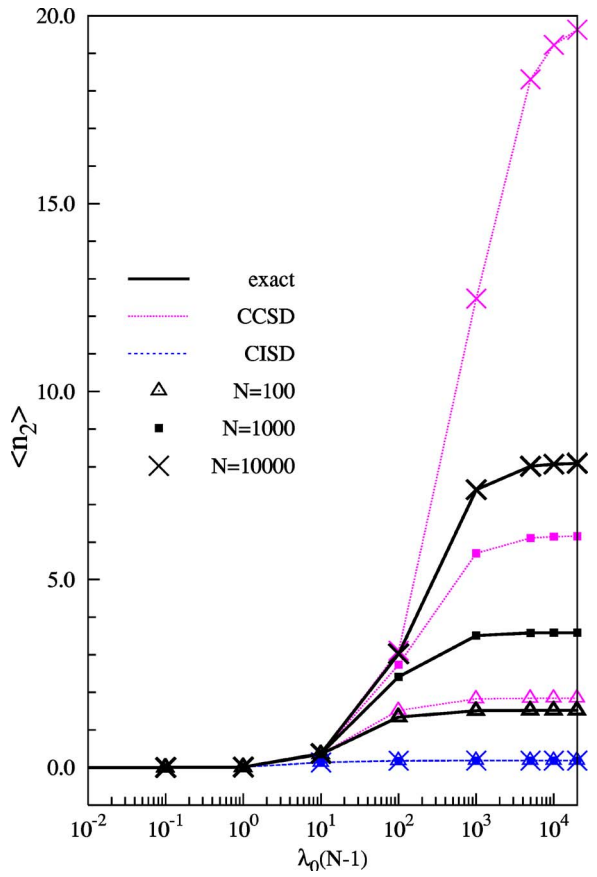

FIG. 3. (Color online) Performance of CCSD method: ground-state depletion. Shown is the average number of bosons in orbital φ_2, $\langle n_2\rangle$, for $N=100, 1000, 10\,000$ bosons and several values of interaction strength. Because of the different spatial symmetry of φ_1 and φ_2, these orbitals are the eigenfunctions of the reduced one-particle density matrix (natural orbitals) and the respective eigenvalues are $\langle n_1\rangle$ and $\langle n_2\rangle$ with $\langle n_1\rangle+\langle n_2\rangle=N$. It is seen that the CCSD is extremely successful in obtaining the depletion $\langle n_2\rangle$, which is a very sensitive measure of the exactness of the many-body wave function, for all N up to a large coupling constant $\lambda=10^2$. The CISD results are also shown for comparison. See text for more details.

obtained with a single parameter c_{22}. The deviations of $\langle n_2\rangle$ for large N and larger interaction strength λ_0 is related to the tail of the C_{2m} distribution. As N and λ_0 increase, there are more and more non-negligible CCSD coefficients which start to deviate from the exact ones. While this does not lead to an error of more than 3% in the correlation energy, see Fig. 1, it does influence the more sensitive measure of exactness of the wave function $\langle n_2\rangle$. For comparison, we also computed the corresponding $\langle n_2\rangle$ values with CISD and plotted the results in Fig. 3. We obtained that the values of $\langle n_2\rangle$ for all N saturates at about 0.18 with increasing λ, which is more than an order of magnitude smaller than the exact and CCSD results. This near independence of $\langle n_2\rangle$ in CISD from the number of bosons N is a manifestation of the minimal correlations embedded in the CISD wave function, in contrast to the CCSD wave function.

Summarizing the results depicted in Figs. 1–3, we see that the CCSD for bosons performs remarkably well even for large interaction strengths. Utilization of the ground configuration in Eq. (7) is an appropriate choice for the coupled-cluster expansion at least for this example (see also the discussion below).

VI. SUMMARY AND CONCLUSIONS

The straightforward configuration-interaction approach rapidly becomes impractical in the many-body problem. When the interaction between N bosons is substantial and/or many of them are present, the number of configurations necessary to correctly describe the correlated wave function quickly increases beyond computational reach. In searching for more efficient approaches which are amenable to systematic approximations (truncations), we have developed in this paper a coupled-cluster theory for systems of bosons in external traps.

In the coupled-cluster approach the exact wave function is obtained by applying an exponential operator $\exp\{T\}$ to the ground configuration $|\phi_0\rangle$. The ground configuration $|\phi_0\rangle$ depends, of course, on the particle statistics. While for fermions it is a determinant with $M=N$ different orbitals, the situation for bosons is more intricate. Since there is no limitation on the number of bosons occupying a certain orbital, there are ample legitimate choices for the ground permanent of N interacting bosons over M available orbitals. The most natural choice for noninteracting or weakly interacting bosons is, of course, to let all bosons reside in the orbital lowest in energy φ_1, $|\phi_0\rangle=\frac{1}{\sqrt{N!}}(b_1^\dagger)^N|0\rangle$, which is our main choice for the coupled-cluster theory presented here.

Because of the simple structure of $|\phi_0\rangle$, the appearance of excitation operators $T=\Sigma_{n=1}^N T_n$ for bosons is much simpler than for fermions. When the simplest truncation $T=T_1$ is chosen, namely, CCS, the effect of $\exp\{T_1\}$ on $|\phi_0\rangle$ is to transform φ_1 to another orbital $\tilde{\varphi}_1$. $\exp\{T_1\}$ optimizes this orbital by mixing the M available orbitals. This reminds us of the situation encountered for fermions, where the operation of the fermionic T_1 transforms the ground determinant into another determinant (Thouless theorem [30]).

In a substantial part of this work we addressed the issue of size consistency for bosons and enquired whether truncated coupled-cluster expansions are size consistent. It turns out that the answer to this question depends on the choice of ground configuration (permanent). Considering R noninteracting replica of the N-boson system, it has been found that truncated coupled-cluster expansions *are not* size consistent with the simplest choice for the R-replica ground permanent $|\phi_0\rangle=\frac{1}{\sqrt{(NR)!}}(b_1^\dagger)^{NR}|0\rangle$, already for the mean-field energy $\langle\phi_0|H|\phi_0\rangle$. This is a surprising result when compared to the case of fermions. Fortunately, this violation of size consistency, at least for the mean-field energy, leads to negligible errors for large individual systems ($N\gg 1$). Can size consistency in bosonic systems be fully restored, perhaps with another choice of the R-replica ground permanent? Yes, it has been straightforwardly shown that truncated coupled-cluster expansions are size consistent with the ground permanent

$|\phi_0\rangle = \frac{1}{(N!)^{R/2}} \Pi_{k=1}^{R} (b_{1_k}^{\dagger})^N |0\rangle$, which "distinguishes" between the R replica; also see discussion below.

Next, we moved to derive working equations of the coupled-cluster approach for the natural ground configuration $|\phi_0\rangle = \frac{1}{\sqrt{N!}} (b_1^{\dagger})^N |0\rangle$. First, it has been shown that the exact correlation energy depends on two kinds of coefficients only: $\{c_k\}$ and $\{c_{kl}\}$ of the single and double excitation operators T_1 and T_2. For a given truncation of the coupled-cluster exponential operator $\exp\{T\}$, it is possible in principle to calculate the correlation energy. Here, for the specific truncation of $T=T_1+T_2$, i.e., CCSD, general working equations for $\{c_k\}$, $\{c_{kl}\}$ have been explicitly derived.

Finally, we tested the performance of the CCSD in a model where an exact solution can be computed. We employed an harmonic trap and restricted the orbital space to two orbitals of different spatial symmetry. The exact solution is obtained, of course, by diagonalizing the many-body Hamiltonian within the full configuration-interaction space spanned by $|m,m'\rangle$, $m=0,\ldots,N, m'=N-m$. In contrast, the CCSD approach requires here one parameter only, c_{22}, which is a solution of a simple algebraic equation of the second degree, see Eq. (58). The performance of the CCSD approach for $N=100, 1000$, and 10 000 interacting bosons was tested in terms of three criteria: correlation energy, many-body wave function, and ground-state depletion. It was found that the CCSD is remarkably successful in obtaining the correlation energy, with absolute error of less than 4% up to a huge coupling constant $\lambda = 2 \times 10^4$, see Fig. 1. The quality of the CCSD many-body wave function and its ability to accurately describe ground-state depletion were found to be remarkably good for all boson numbers and coupling constants as large as $\lambda = 10^2$, see Figs. 2 and 3. For comparison, we examined the performance of CISD, which similarly depends on one parameter only d_{22}. CISD was found to be substantially poorer in comparison to CCSD. For instance, it accounts for about 50% of the correlation energy only.

The coupled-cluster theory for bosons presented in this work, as certainly supported by the numerical example, is a promising approach to be further developed in the many-boson problem. The expressions of the bosonic coupled-cluster theory are much simpler than those for fermions since, generally, the ground configuration (permanent) employs one orbital only. Consequently, we can treat a very large number of bosons with coupled-cluster expansions and employ more virtual (nonoccupied) orbitals than the fermionic coupled-cluster can. These qualities open the way to study few- to many-boson systems up to a substantial interaction where several orbitals are needed to describe the reality.

The issue of size consistency, as extensively discussed above, is delicate for bosons, and depends on the choice of the ground configuration. It relates to the following practical point: what is a suitable choice of the ground permanent when a coupled-cluster expansion is to be employed with a specific physical system? We can say that, for bosons in a single-well trap an useful choice is the simplest permanent where all bosons reside in the same orbital, which is the standard mean-field GP orbital. However, if we wish to usefully apply coupled-cluster expansions to a bosonic system undergoing spatial fragmentation or superfluid to Mott-insulator transitions, situations that occur in double-well and multiple-well traps, we have to be more careful with the choice of ground configuration, and depart from the simplest permanent constructed from the GP mean-field orbital. Recently, a more general mean-field theory has been introduced, allowing for bosons to reside in several orbitals [28]. We anticipate that in combination with coupled-cluster expansions they can be useful for studying many bosons in double-well and multiple-well traps.

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APPENDIX

The transformed two-body operator $\dot{V}$ of the transformed Hamiltonian $\dot{H}=\dot{H}_0+\dot{V}$ consists of the nine terms listed below.

$$\dot{V} = \sum_{p=1}^{9} \dot{V}(p),$$

$$\dot{V}(1) = \frac{1}{2} V_{1111} \dot{b}_1^{\dagger} \dot{b}_1^{\dagger} b_1 b_1,$$

$$\dot{V}(2) = \sum_{k=2}^{M} V_{111k} \dot{b}_1^{\dagger} \dot{b}_1^{\dagger} b_1 \dot{b}_k,$$

$$\dot{V}(3) = \sum_{k=2}^{M} V_{k111} b_k^{\dagger} \dot{b}_1^{\dagger} b_1 b_1,$$

$$\dot{V}(4) = \frac{1}{2} \sum_{k,l=2}^{M} V_{11kl} \dot{b}_1^{\dagger} \dot{b}_1^{\dagger} \dot{b}_k \dot{b}_l,$$

$$\dot{V}(5) = \frac{1}{2} \sum_{k,l=2}^{M} V_{kl11} b_k^{\dagger} b_l^{\dagger} b_1 b_1,$$

$$\dot{V}(6) = \sum_{k,l=2}^{M} \left(V_{1k1l} + V_{1kl1}\right) \dot{b}_1^{\dagger} b_k^{\dagger} b_1 \dot{b}_l,$$

$$\dot{V}(7) = \sum_{j,k,l=2}^{M} V_{1jkl} \dot{b}_1^{\dagger} b_j^{\dagger} \dot{b}_k \dot{b}_l,$$

$$\dot{V}(8) = \sum_{j,k,l=2}^{M} V_{jkl1} b_j^{\dagger} b_k^{\dagger} \dot{b}_l b_1,$$

$$\dot{V}(9) = \frac{1}{2} \sum_{i,j,k,l=2}^{M} V_{ijkl} b_i^{\dagger} b_j^{\dagger} \dot{b}_k \dot{b}_l.$$

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