Ground state of charged bosons confined in a harmonic trap

Yeong E. Kim* and Alexander L. Zubarev†
Department of Physics, Purdue University, West Lafayette, Indiana 47907

(Received 13 November 2000; revised manuscript received 7 March 2001; published 30 May 2001)

We study a system composed of N identical charged bosons confined in a harmonic trap. Upper- and lower-energy bounds are given. It is shown in the large-N limit that the ground-state energy is determined within an accuracy of $\pm 8\%$ and that the mean-field theory provides a reasonable result with a relative error of less than 16% for the binding energy.

DOI: 10.1103/PhysRevA.64.013603 PACS number(s): 03.75.Fi, 05.30.Jp

I. INTRODUCTION

We study a system composed of N identical bosons interacting via the Coulomb repulsive force that are confined in an isotropic harmonic trap.

Investigations of charged Bose gases have been reported in a number of papers [1–7]. In a recent paper [6], the mean-field theory for bosons in the form given in Ref. [8] was used to describe the ground state of a bosonic Thomson atom. The equivalence of the Coulomb systems in a harmonic trap to the Thomson atom model [9] was discussed in Refs. [6,10,11]. The model approximately simulates a number of physical situations such as systems of ions in a three-dimensional trap (radiofrequency or Penning trap) [10,11], electrons in quantum dots [12,13], etc.

Since no exact general solution of the N-body problem has been found, to investigate the validity of the mean-field approximation for the case of systems of charged bosons confined in a trap, we propose in this paper to compare the mean-field energy with lower and upper bounds. Such an approach was used to establish the asymptotic accuracy of the Ginzburg-Pitaevskii-Gross ground-state energy for dilute neutral Bose gas with repulsive interaction [14].

We find that our lower and upper bounds provide the actual value of ground-state energy within $\pm 8\%$ accuracy. We also show that, for the case of large N, the mean-field theory is a reasonable approximation with a relative error of less than 16% for the binding energy.

The paper is organized as follows. In Sec. II, we describe an outline of the mean-field method. Energy and single-particle density are found analytically in the large-N limit. In Sec. III, we generalize a lower-bound method developed by Post and Hall [15] for the case of charged bosons confined in a harmonic trap. In Sec. IV, we describe the strong-coupling perturbative expansion method. In Sec. V, we describe our calculation of upper bounds using the effective linear two-body equation (ELTBE) method [16]. In Sec. VI, we consider the Wigner-crystallization regime. A summary and conclusions are given in Sec. VII.

II. MEAN-FIELD METHOD

To describe ground-state properties of a system of interacting bosons confined in a harmonic trap, we start from the mean-field theory for bosons in the following form given in Ref. [8]:

$$\left(-\frac{\hbar^2}{2m}\Delta + V_t(\vec{r}) + (N-1)V_H(\vec{r})\right)\Psi(\vec{r}) = \mu\Psi(\vec{r}), \quad (1)$$

where $\Psi(\vec{r})$ is the normalized ground-state wave function, $V_t(\vec{r}) = m\omega^2 r^2/2$ is a harmonic trap potential with $r^2 = x^2 + y^2 + z^2$, $V_H(\vec{r}) = \int d\vec{r} V_{\rm int}(\vec{r}-\vec{r}\,')|\Psi(\vec{r}\,')|^2$ is the Hartree potential with an interacting potential $V_{\rm int}(\vec{r})$, and N is the number of particles in a trap. The chemical potential μ is related to the mean-field ground-state energy E_M and particle number N by the general thermodynamic identity

$$\mu = \frac{\partial E_M}{\partial N} \quad (2)$$

for $N \to \infty$, where the mean-field ground-state energy E_M is given by

$$E_M = N\left(\langle\Psi| -\frac{\hbar^2}{2m}\Delta|\Psi\rangle + \langle\Psi|V_t|\Psi\rangle + \frac{N-1}{2}\langle\Psi|V_H|\Psi\rangle\right). \quad (3)$$

We note that the mean-field theory, Eq. (1), cannot describe the Wigner-crystallization regime [17] (see also Ref. [6]).

We introduce dimensionless units by making the following transformations: (i) $\vec{r} \to a\vec{r}$, where $a = \sqrt{\hbar/(m\omega)}$, and (ii) the energy and chemical potential are measured in units of $\hbar\omega$.

Using the above dimensionless notation, we can rewrite Eq. (1) as

$$\left(-\tfrac{1}{2}\Delta + \frac{r^2}{2} + (N-1)\int d\vec{r}\,' V_{\rm int}(\vec{r}-\vec{r}\,')|\Psi(\vec{r}\,')|^2\right)\Psi(\vec{r}) = \mu\Psi(\vec{r}). \quad (4)$$

In the limit $N \gg 1$, the nonlinear Schrödinger equation (4) can be simplified by omitting the kinetic energy, yielding the following integral equation:

$$\frac{r^2}{2} + N\int d\vec{r}\,' V_{\rm int}(\vec{r}-\vec{r}\,')|\Psi(\vec{r}\,')|^2 = \mu, \quad (5)$$

where $r^2 < 2\tilde{\mu}$ and $|\Psi(\vec{r})|^2 = 0$; if $r^2 > 2\tilde{\mu}$, $\tilde{\mu}$ is to be determined from the minimum of the energy functional,

*Email address: yekim@physics.purdue.edu
†Email address: zubareva@physics.purdue.edu

$$E_M=\frac{N}{2}\int|\Psi(\vec{r})|^2r^2d\vec{r}+\frac{N^2}{2}\int|\Psi(\vec{r})|^2|\Psi(\vec{r}\,')|^2V_{\rm int}(\vec{r}-\vec{r}\,')d\vec{r}\,d\vec{r}\,'.$$

This method [Eq. (5)] is another possible implementation of the Thomas-Fermi treatment of neutral, dilute vapors [18,19]. For review of the Thomas-Fermi theory of atoms, see Ref. [20].

To make a proper choice for the large-N limit of the Hamiltonian for bosons interacting via the Coulomb potential

$$V_{\rm int}(r)=\frac{\gamma_c}{r} \tag{6}$$

with $\gamma_c=Z^2\alpha\sqrt{mc^2/(\hbar\omega)}>0$, we rescale variables $\vec{r}=(N\gamma_c)^{1/3}\vec{z}$. Now we can rewrite Eq. (4) as

$$\left(-\frac{\epsilon}{2}\Delta+\frac{z^2-R^2}{2}+\int\frac{d\vec{z}\,'}{|\vec{z}-\vec{z}\,'|}|\Psi(\vec{z}\,')|^2\right)\Psi(\vec{z})=0, \tag{7}$$

where $R^2=2\mu/(N\gamma_c)^{2/3}$, $\epsilon=1/(N\gamma_c)^{4/3}$, and $N\gg1$.

In the case $N\gamma_c\gg1$, the solution of Eq. (5) is found to be

$$|\Psi(\vec{r})|^2=\frac{3}{4\pi N\gamma_c}\theta(2\tilde{\mu}-r^2), \tag{8}$$

where θ denotes the unit positive step function, and

$$\tilde{\mu}=\frac{\mu}{3}. \tag{9}$$

Straightforward calculations with $|\Psi(\vec{r})|^2$ from Eq. (8) yield

$$\mu=\tfrac{3}{2}(\gamma_cN)^{2/3},\qquad E_M=\tfrac{9}{10}(\gamma_c)^{2/3}N^{5/3}. \tag{10}$$

Equation (8) is obtained by neglecting the $(\epsilon/2)\Delta\,\Psi$ term in Eq. (7) and provides an accurate description of the exact solution where the gradients of the wave function are small. In a boundary layer of a narrow region near surface, the approximation (8) breaks down. We expect that the thickness of this boundary layer approaches zero as $\epsilon\to0$. Recent numerical calculations [6] support our analytical results. Equation (10) provides an upper bound for the ground-state energy in the large-N limit ($N\gg1$ and $N\gamma_c\gg1$).

III. LOWER BOUNDS

In this section, we consider N identical charged bosons confined in a harmonic isotropic trap with the following Hamiltonian:

$$H=-\tfrac{1}{2}\sum_{i=1}^{N}\Delta_i+\tfrac{1}{2}\sum_{i=1}^{N}r_i^2+\sum_{i<j}V_{ij}, \tag{11}$$

where

$$V_{ij}=\frac{\gamma_c}{|\vec{r}_i-\vec{r}_j|}. \tag{12}$$

Now we introduce the Jacobi coordinates $\vec{\zeta}_1=\vec{R}=(1/N)\Sigma_{i=1}^N\vec{r}_i$, the center-of-mass coordinate, and ($i\geqslant2$)

$$\vec{\zeta}_i=\frac{1}{\sqrt{i(i-1)}}\left((1-i)\vec{r}_i+\sum_{k=1}^{i-1}\vec{r}_k\right). \tag{13}$$

Using

$$\sum_{i=1}^{N}r_i^2=NR^2+\sum_{i=2}^{N}\zeta_i^2, \tag{14}$$

we can rewrite Eq. (11) as

$$H=-\frac{1}{2N}\Delta_R-\tfrac{1}{2}\sum_{i=2}^{N}\Delta_{\zeta_i}+\tfrac{1}{2}NR^2+\tfrac{1}{2}\sum_{i=2}^{N}\zeta_i^2+\sum_{i<j}V_{ij}. \tag{15}$$

Hence we have for the ground-state energy

$$E=\tfrac{3}{2}+\langle\psi|\left(-\tfrac{1}{2}\sum_{i=2}^{N}\Delta_{\zeta_i}+\tfrac{1}{2}\sum_{i=2}^{N}\zeta_i^2+\sum_{i<j}V_{ij}\right)|\psi\rangle, \tag{16}$$

where $\psi(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)$ is the ground-state wave function. Using symmetric properties of ψ, we can rewrite Eq. (16) as

$$E=\tfrac{3}{2}+\langle\psi|(N-1)\left(-\tfrac{1}{2}\Delta_{\zeta_2}+\tfrac{1}{2}\zeta_2^2+\frac{N}{2}V_{12}(\sqrt{2}\zeta_2)\right)|\psi\rangle. \tag{17}$$

Projecting $|\psi\rangle$ on the complete basis $|n\rangle$, generated by the effective two-body eigenvalue problem

$$H^{(0)}|n\rangle=(N-1)\left[-\tfrac{1}{2}\Delta_{\zeta_2}+\tfrac{1}{2}\zeta_2^2+\frac{N}{2}V_{12}(\sqrt{2}\zeta_2)\right]|n\rangle=\epsilon_n|n\rangle, \tag{18}$$

we get

$$E=\tfrac{3}{2}+\sum_n\epsilon_n|\langle\psi|n\rangle|^2\geqslant(\tfrac{3}{2}+\epsilon_0). \tag{19}$$

Hence the ground-state energy of the effective two-body Hamiltonian $H^{(0)},\epsilon_0$ is a lower bound of $E-\tfrac{3}{2}$. Equation (19) is a generalization of the Post and Hall lower-bound method [15] for the case of a system of interacting particles confined in a harmonic trap. In the particular case of bosons with the Hooke interaction, this procedure, Eq. (19), gives the exact value of the ground-state energy (see the Appendix for details).

To find ϵ_0 for the Coulomb interaction case, Eq. (6), we need to solve the effective two-body problem,

$$\tilde{H}\phi=-\frac{1}{2}\frac{d^2\phi}{d\zeta^2}+\tfrac{1}{2}\zeta^2\phi+\frac{\lambda}{\zeta}\phi=\tilde{\epsilon}\phi, \tag{20}$$

where $\lambda=N\gamma_c/(2\sqrt{2})$ and $\tilde{\epsilon}=\epsilon_0/(N-1)$.

For the case of $\lambda<1$, the weak-coupling-perturbation (WCP) calculation leads to the ground-state energy $\tilde{\epsilon}$ given by [24]

$$\tilde{\epsilon}=\tfrac{3}{2}+1.128\,379\lambda-0.155\,78\lambda^2+\cdots. \tag{21}$$

IV. STRONG-COUPLING PERTURBATIVE EXPANSION

The two-body problem with the so-called spiked harmonic oscillator (SHO) $V(r)=r^2+[l(l+1)/r^2]+(\lambda/r^{\alpha})$, where $r\geqslant 0$ and α is positive constant, has been the subject of intensive study [21–28]. The quantity λ is a positive-definite parameter that measures the strength of the perturbative potential. It was found [22] that the normal perturbation theory could not be applied for the values $\alpha\geqslant\frac{5}{2}$, the so-called singular spiked harmonic oscillator. In Ref. [21], a special perturbative theory was developed for this case. A strong-coupling perturbative expansion (SCP) $(\lambda>1)$ was carried out in Ref. [24]. In Ref. [27], the SCP was used for the case of $\alpha=3$. In Refs. [23,26], it was shown that the SHO problem with $\alpha=1$ is solvable analytically for a particular set of oscillator frequencies. For example, for $\lambda=1$ we have [23]

$$\tilde{\epsilon}=\tfrac{5}{2},\quad \phi(\zeta)=\zeta e^{-\zeta^2/2}(1+\zeta), \tag{22}$$

and for $\lambda=\sqrt{5}$ we have [26]

$$\tilde{\epsilon}=\tfrac{7}{2},\quad \phi(\zeta)=\zeta e^{-\zeta^2/2}(1+\sqrt{5}\zeta+\zeta^2). \tag{23}$$

Equation (20) can be solved for the case of large λ using the SCP [24]. The idea of this method is to expand the potential $V(\zeta)=(\zeta^2/2)+(\lambda/\zeta)$ around its minimum,

$$V(\zeta)=\tfrac{3}{2}\lambda^{2/3}+\tfrac{3}{2}(\zeta-\lambda^{1/3})^2+\sum_{i=1}^{\infty}(-1)^i\frac{\lambda^{-i/3}}{i+2}(\zeta-\lambda^{1/3})^{i+2}. \tag{24}$$

Substitution of Eq. (24) into Eq. (20) gives

$$\tilde{H}=H_0+H', \tag{25}$$

where the nonpertubative Hamiltonian H_0 is given by

$$H_0=-\frac{1}{2}\frac{d^2}{dz^2}+\tfrac{3}{2}\lambda^{2/3}+\tfrac{3}{2}z^2 \tag{26}$$

and the pertubation H' is given by

$$H'=\sum_{i}^{\infty}H_i\lambda^{-i/3}, \tag{27}$$

with $H_i=(-1)^i z^{i+2}/(i+2)$ and $z=(\zeta-\lambda^{1/3})$.

Now ϕ and $\tilde{\epsilon}$ can be written as

$$\phi=\lim_{n\to\infty}\phi_n \tag{28}$$

and

$$\tilde{\epsilon}=\lim_{n\to\infty}\tilde{\epsilon}_n, \tag{29}$$

where $\phi_n=\Sigma_{i=0}^{n}\phi^{(i)}\lambda^{-i/3}$ and $\tilde{\epsilon}_n=\Sigma_{i=0}^{n}\tilde{\epsilon}^{(i)}\lambda^{-i/3}$. Substituting Eqs. (26), (28), and (29) into Eq. (20) gives

$$\sum_{i=0}^{n}H_i\phi^{(n-i)}=\sum_{i=0}^{n}e^{(i)}\phi^{(n-i)}. \tag{30}$$

The complete oscillator basis $|\tilde{n}\rangle$, $H_0|\tilde{n}\rangle=e_n|\tilde{n}\rangle$, where $z=(\zeta-\lambda^{1/3})$ is extended to the full real axis, is used to solve Eq. (30) with $e_0=\tilde{\epsilon}^{(0)}$ and $|0\rangle=\phi^{(0)}$. We note that the region $-\infty<z\leqslant-\lambda^{1/3}$ is spurious. For large λ, it is expected that the harmonic-oscillator basis does not penetrate too much into the forbidden region $z<-\lambda^{1/3}$. From Table I, we can see that the SCP converges very fast for $\lambda>2$. However, for the case of $\lambda=1$, it is certainly outside the convergence radius (see Table II). Even in this case, $\tilde{\epsilon}_0$ is still a good lower approximation for $\tilde{\epsilon}$.

From the SCP expansion in the large-λ limit, we obtain in the large-N limit ($N\gg 1$ and $N\gamma_c\gg 1$)

$$\epsilon_0=\tfrac{3}{4}N^{5/3}\gamma_c^{2/3}. \tag{31}$$

Combining Eq. (31) with Eq. (10), we get in this limit

$$\tfrac{3}{4}N^{5/3}\gamma_c^{2/3}\leqslant E\leqslant\tfrac{9}{10}N^{5/3}\gamma_c^{2/3}, \tag{32}$$

where E is the leading term of the ground-state energy. Hence the leading term of the ground-state energy in the large-N limit is determined within an accuracy of $\pm 8\%$. We can therefore state that the mean-field theory, Eq. (10), provides a reasonable result in this limit for the ground-state energy.

TABLE I. Results for ground-state energy, $\tilde{\epsilon}$ [Eq. (20)]. We compare zero-order, second-order, and converged results (10th order) to the exact analytical solution [Eqs. (22) and (23)].

λ	$\tilde{\epsilon}_0$	$\tilde{\epsilon}_2$	$\tilde{\epsilon}_{\text{converged}}$	$\tilde{\epsilon}_{\text{exact}}$
1	2.36603	2.46325		2.5
$\sqrt{5}$	3.43099	3.48785	3.49954	3.5
10	7.82841	7.84935	7.85061	
100	33.18255	33.18705	33.18711	
500	95.3601	95.36165	95.36165	
1000	150.86603	150.86700	150.86700	
5000	439.46869	439.46902	439.46902	
10000	697.10435	697.10456	697.10456	

TABLE II. Results for $\tilde{\epsilon}_n$ for the $\lambda=1$ case.

λ	$\tilde{\epsilon}_0$	$\tilde{\epsilon}_2$	$\tilde{\epsilon}_4$	$\tilde{\epsilon}_6$	$\tilde{\epsilon}_8$	$\tilde{\epsilon}_{10}$
1	2.36603	2.46325	2.48797	2.49716	2.50439	2.5125

V. UPPER BOUNDS

Our method for obtaining the upper bounds, the equivalent linear two-body equation (ELTBE) method [16], consists of two steps. The first is to give the N-body wave function $\psi(\vec{r}_1,\vec{r}_2,\ldots)$ a particular functional form,

$$\psi(\vec{r}_1,\ldots,\vec{r}_N)\approx\frac{\Phi(\rho)}{\rho^{(3N-1)/2}}, \tag{33}$$

where $\rho=[\sum_{i=1}^{N}r_i^2]^{1/2}$.

The second step is to derive an equation for $\Phi(\rho)$ by requiring that $\psi(\vec{r}_1,\vec{r}_2,\ldots)$ must satisfy a variational principle $\delta\langle\psi|H|\psi\rangle=0$ with a subsidiary condition $\langle\psi|\psi\rangle=1$. H is the Hamiltonian. This leads to the following equation:

$$H_\rho\Phi=\left(-\frac{1}{2}\frac{d^2}{d\rho^2}+\tfrac{1}{2}\rho^2+\frac{(3N-1)(3N-3)}{8\rho^2}+\frac{\tilde{\lambda}}{\rho}\right)\Phi=\tilde{E}\Phi, \tag{34}$$

where

$$\tilde{\lambda}=\frac{2}{3\sqrt{2\pi}}\gamma_c N\frac{\Gamma(3N/2)}{\Gamma(3N/2-3/2)}. \tag{35}$$

The lowest eigenvalue of H_ρ [Eq. (34)] is an upper bound of the lowest eigenvalue of the original N-body problem. Since a variational estimate of the lowest eigenvalue of H_ρ is also an upper bound of the ground-state energy of the original N-body problem, we have for this upper bound, E_{upper}, the following expression:

$$E_{\text{upper}}=\frac{\langle\Phi_t|H_\rho|\Phi_t\rangle}{\langle\Phi_t|\Phi_t\rangle}. \tag{36}$$

Assuming the form for the trial function Φ_t,

$$\Phi_t(\rho)=\rho^{(3N-1)/2}e^{-\rho^p/(2\alpha^p)}, \tag{37}$$

we obtain

$$E_{\text{upper}}=\frac{p(3N-2+p)\Gamma[(3N-2)/p+1]}{8\Gamma(3N/p)\alpha^2}+\frac{\Gamma[(3N+2)/p]}{2\Gamma(3N/p)}\alpha^2+\frac{\tilde{\lambda}\Gamma[(3N-1)/p]}{\Gamma(3N/p)\alpha}, \tag{38}$$

where parameters α and p are to be determined from a solution of the following equations:

$$\frac{\partial E_{\text{upper}}}{\partial\alpha}=\frac{\partial E_{\text{upper}}}{\partial p}=0. \tag{39}$$

From Table III, we can see that for the case of $N\gamma_c\leqslant 100$, the calculated bounds determine the actual value of the ground-state energy within $\pm\Delta$ accuracy, with $\Delta<9\%$.

TABLE III. Results for upper, E_{upper}/N, and lower, E_{lower}/N, bounds of ground-state energy per particle, and $\Delta=(E_{\text{upper}}-E_{\text{lower}})/(2E_{\text{upper}})$.

N	$\lambda=N\gamma_c/(2\sqrt{2})$	E_{lower}/N	E_{upper}/N	Δ (%)
10	0.1	1.60015	1.60048	0.02
	0.5	1.97272	1.98724	0.4
	1	2.4	2.43945	0.8
	$\sqrt{5}$	3.3	3.4478	2.1
	10	7.21555	8.18751	5.9
	100	30.0184	36.8931	9.3
100	0.1	1.61017	1.61068	0.02
	0.5	2.01999	2.03468	0.36
	1	2.49	2.52904	0.8
	$\sqrt{5}$	3.48	3.62737	2.0
	10	7.7871	8.76512	5.6
	100	32.8702	39.8116	8.7

VI. LARGE γ_c LIMIT

To make a proper choice for the large-γ_c limit of the Hamiltonian, Eq. (11), we rescale variables, $\vec{r}\to\gamma_c^{1/3}\vec{r}$, and write the Schrödinger equation for N identical charged bosons confined in a harmonic isotropic trap as

$$\left(-\frac{1}{2\gamma_c^{(4/3)}}\sum_{i=1}^{N}\Delta_i+\tfrac{1}{2}\sum_{i=1}^{N}r_i^2+\sum_{i<j}\frac{1}{|\vec{r}_i-\vec{r}_j|}\right)\psi=\frac{E}{\gamma_c^{2/3}}\psi. \tag{40}$$

Equation (40) describes the motion of N particles with an effective mass $\gamma_c^{4/3}$. Therefore, when $\gamma_c\to\infty$, the effective mass of the particles becomes infinitely large and then the particles may be assumed to remain essentially stationary at the absolute minimum of the potential energy,

$$V_{\text{eff}}(\vec{r}_1,\ldots,\vec{r}_N)=\tfrac{1}{2}\sum_{i=1}^{N}r_i^2+\sum_{i<j}\frac{1}{|\vec{r}_i-\vec{r}_j|}, \tag{41}$$

with quantum fluctuations around the classical minimum. Obviously, this assumption fails if the potential energy V_{eff} does not possess a minimum and (or) gradients of the wave functions are large. This large-γ_c limit is the Wigner crystallization regime [6].

Interest in the investigation of the Wigner-crystallized ground state has grown as a result of a recently proposed quantum computer by Cirac and Zoller [29]. (See also Refs. [30–33].)

As we have already noted in Sec. II, mean-field theory, Eq. (1), cannot describe the crystallized ground state. Therefore, we can only state that the mean-field ground-state energy is an upper bound to the exact energy. Straightforward calculations for the case of $\gamma_c\gg 1$ give the Thomas-Fermi upper bound

$$E_{\text{upper}}=\tfrac{9}{10}N[\gamma_c(N-1)]^{2/3}. \tag{42}$$

From the SCP expansion, Eq. (24), we obtain in the large-γ_c limit a lower bound

$$E_{\rm low}=\epsilon_0=\tfrac{3}{4}(N-1)(N\gamma_c)^{2/3}. \tag{43}$$

Therefore, for the leading term of the ground-state energy, E, we have

$$\tfrac{3}{4}(N-1)(N\gamma_c)^{2/3}\leqslant E\leqslant \tfrac{9}{10}N[\gamma_c(N-1)]^{2/3}. \tag{44}$$

From Eq. (44), we can see that in the case of the Wigner-crystallization regime, $\gamma_c\gg 1$, our bounds determine the ground-state energy within $\pm\Delta$ accuracy, with $\Delta\approx 8\%$ for $N\geqslant 100$, $\Delta\approx 10\%$ for $N=10$, and $\Delta\approx 15\%$ for $N=3$. It shows that the mean-field theory, Eq. (10), provides a reasonable upper bound for $N>10$ even in the large-γ_c limit. However, the Thomas-Fermi treatment cannot describe the crystallized ground-state wave function, since a small relative error of the mean-field ground-state energy does not necessarily imply that the mean-field (product) state describes the actual many-body wave function well.

VII. SUMMARY AND CONCLUSION

In summary, we have generalized the Post and Hall lower-bound method [15] for the case of interacting bosons confined in a harmonic trap.

As examples of application, we have studied bosons interacting with Coulomb forces in a harmonic trapping potential. We have found the upper bounds using the mean-field approach and the ELTBE method [16].

It is shown that the leading term of the ground-state energy in the large-N limit ($N\gg 1$ and $N\gamma_c\gg 1$) is determined within an accuracy of $\pm 8\%$, and it is also shown that the mean-field theory provides reasonable results with a relative error of less than 16% for the leading term of the ground-state energy.

However, the Thomas-Fermi treatment cannot describe the crystallized ground-state wave function, since a small relative error of the mean-field ground-state energy does not necessarily imply that the mean-field (product) state describes the actual many-body wave function well.

APPENDIX

In this appendix, we consider the Hamiltonian [34,35]

$$H=-\tfrac{1}{2}\sum_{i=1}^{N}\Delta_i+\tfrac{1}{2}\sum_{i=1}^{N}r_i^2+\frac{\Lambda}{2}\sum_{i<j}(\vec r_i-\vec r_j)^2, \tag{A1}$$

which was used for a problem in nuclear physics in Ref. [36].

Using Eq. (14) and

$$\sum_{i<j}(\vec r_i-\vec r_j)^2=N\sum_{i=2}^{N}\zeta_i^2, \tag{A2}$$

we can rewrite Eq. (A1) as

$$H=-\frac{1}{2N}\Delta_R+\tfrac{1}{2}NR^2+\sum_{i=2}^{N}\left(-\tfrac{1}{2}\Delta_{\zeta_i}+\frac{1+N\Lambda}{2}\zeta_i^2\right). \tag{A3}$$

This leads to the ground-state energy

$$E=\tfrac{3}{2}[1+\sqrt{1+N\Lambda}(N-1)], \tag{A4}$$

which is equal to the lower bound, Eq. (19), with

$$\epsilon_0=\tfrac{3}{2}\sqrt{1+N\Lambda}(N-1). \tag{A5}$$

[1] M. F. M. Osborne, Phys. Rev. **76**, 400 (1949).
[2] M. R. Schafroth, Phys. Rev. **100**, 463 (1955).
[3] L. L. Foldy, Phys. Rev. **124**, 649 (1961).
[4] K. A. Brueckner, Phys. Rev. **156**, 204 (1967).
[5] A. S. Alexandrov, W. H. Beere, and V. V. Kabanov, Phys. Rev. B **54**, 15 363 (1996).
[6] T. Schneider and R. Blümel, J. Phys. B **32**, 5017 (1999).
[7] A. Gonzales, B. Partoens, A. Matulis, and F. M. Peeters, Phys. Rev. B **59**, 1653 (1999).
[8] B. D. Esry, Phys. Rev. A **55**, 1147 (1997).
[9] J. J. Thomson, Philos. Mag. **7**, 237 (1904).
[10] Yu. E. Lozovik, Usp. Fiz. Nauk. **153**, 356 (1987) [Phys. Usp. **30**, 912 (1987)].
[11] F. Diedrich, E. Peik, J. M. Chen, W. Quint, and H. Walter, Phys. Rev. Lett. **59**, 2931 (1987); D. J. Wineland, J. C. Bergquist, W. M. Itano, J. J. Bolinger, and C. H. Manney, *ibid.* **59**, 2935 (1987).
[12] M. A. Read and W. P. Kirk, *Nanostructure Physics and Fabrication* (Academic, Boston, 1989); L. Jacak, P. Hawrylak, and A. Wojs, *Quantum Dots* (Springer, Berlin, 1998); T. Chakraborty, *Quantum Dots* (Elsevier, Amsterdam, 1999); D. Bimberg, M. Grundmann, and N. N. Ledentsov, *Quantum Dot Heterostructures* (Wiley, Chichester, 1999).
[13] M. A. Kastner, Phys. Today **46(1)**, 24 (1993).
[14] E. H. Lieb, R. Seiringer, and J. Yngvason, Phys. Rev. A **61**, 043602 (2000).
[15] H. R. Post, Proc. Phys. Soc., London, Sect. A **69**, 936 (1956); H. R. Post, Proc. Phys. Soc. London **79**, 819 (1961); R. L. Hall and H. R. Post, Proc. Phys. Soc. London **90**, 381 (1967).
[16] A. L. Zubarev and Y. E. Kim, Phys. Lett. A **263**, 33 (1999); Y. E. Kim and A. L. Zubarev, J. Phys. B **33**, 55 (2000).
[17] E. P. Wigner, Phys. Rev. **46**, 1002 (1934).
[18] D. A. Huse and E. D. Siggia, J. Low Temp. Phys. **46**, 137 (1982).
[19] G. Baym and C. J. Pethick, Phys. Rev. Lett. **76**, 6 (1996).
[20] E. Lieb, Rev. Mod. Phys. **53**, 603 (1981).
[21] E. M. Harrell, Ann. Phys. (N.Y.) **105**, 379 (1977).
[22] L. C. Detwiler and J. R. Klauder, Phys. Rev. D **11**, 1436 (1975); J. R. Klauder, Science **199**, 735 (1978).
[23] S. Kais, D. R. Hershbach, and R. D. Levine, J. Chem. Phys. **91**, 7791 (1989).
[24] V. C. Aguilera-Navarro, G. A. Esterez, and R. Guardiola, J. Math. Phys. **31**, 99 (1990); V. C. Aguilera-Navarro and R. Guardiola, *ibid.* **32**, 2135 (1991).

[25] M. Znoil, Phys. Lett. A **158**, 436 (1991).
[26] M. Taut, Phys. Rev. A **48**, 3561 (1993).
[27] D. K. Watson and B. A. McKinney, Phys. Rev. A **59**, 4091 (1999).
[28] R. L. Hall and N. Saad, J. Phys. A **33**, 5531 (2000).
[29] J. I. Cirac and P. Zoller, Phys. Rev. Lett. **74**, 4094 (1995).
[30] A. Steane, Appl. Phys. B: Lasers Opt. **64**, 623 (1977).
[31] Phys. World **11(3)**, 33 (1998), special issue on quantum information.
[32] D. F. V. James, Appl. Phys. B: Lasers Opt. **66**, 181 (1998).
[33] A. Sørensen and K. Mølmer, Phys. Rev. Lett. **82**, 1971 (1999).
[34] H. R. Post, Proc. Phys. Soc., London, Sect. A **66**, 649 (1953).
[35] N. F. Johnson and M. C. Payne, Phys. Rev. Lett. **67**, 1157 (1991); A. L. Zubarev and V. B. Mandelzweig, Phys. Rev. C **50**, 38 (1994); F. Brosens, J. T. Devreese, and L. F. Lemmens, Phys. Rev. E **55**, 6795 (1997); N. K. Wilkin, J. M. Gunn, and R. A. Smith, Phys. Rev. Lett. **80**, 2265 (1998).
[36] S. Gartenhaus and C. Schwartz, Phys. Rev. **108**, 482 (1957).