Ground-state properties of bosons in three- and two-dimensional traps

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We study trapped systems of bosons at zero temperature in three and two dimensions. Conditions are fulfilled for the application of Gross-Pitaevskii theory with a positive scattering length. Series expansions for ground-state properties are obtained in both the noninteracting and the strong-coupling (Thomas-Fermi) limits. From these expansions, analytic estimates are presented in the form of two-point Padé approximants. We explicitly show the approximants for the total energy per particle and the chemical potential.

Since the discovery of Bose-Einstein condensation in alkali-vapour atoms, trapped bosonic systems have attracted a lot of attention. In the experiments, the number of confined atoms, $N$, ranges between $10^4$ and $10^9$, whereas the ratio between the scattering length and the harmonic oscillator length is $a/a_{ho} \sim 10^{-3}$, thus the conditions for the application of the Gross-Pitaevskii (GP) theory are fulfilled. We assume that the interaction between pairs of atoms is repulsive, i.e. $a > 0$, as for $^{87}$Rb. The temperature is taken to be zero, that is we are dealing with ground-state properties.

The GP equation for the condensate function, $\psi$, in three dimensions is written as

$$\left\{ \frac{\hbar^2}{2m} \Delta + V_{\text{ext}}(\vec{r}) + g|\psi|^2(\vec{r}) - \mu \right\} \psi = 0,$$

where $m$ is the mass of the atoms, $\mu$ – the chemical potential, and $g = 4\pi \hbar^2 a/m$. The condensate function satisfies the constraint

$$\int d^3r \ |\psi|^2 = N.$$

In (1-2), we have neglected any effect coming from particles out of the condensate. $V_{\text{ext}}(\vec{r})$ is the external potential responsible for the confinement of the atoms. For simplicity, we will study an isotropic trap, that is $V_{\text{ext}} = \frac{1}{2}m\omega^2 r^2$, and $\psi$ is a symmetric function $\psi(\vec{r}) = \psi(r)$.

A scaling of variables, $r \rightarrow a_{ho} r$, $\psi \rightarrow (N/a_{ho}^3)^{1/2} \psi$, $\mu \rightarrow \hbar \omega \mu$, reduces eqs. (1,2) to the dimensionless form

$$\left\{ -\frac{1}{2} \Delta + \frac{1}{2} r^2 + \tilde{g}|\psi|^2 - \mu \right\} \psi = 0,$$

$$\int d^3r \ |\psi|^2 = 1,$$

and makes explicit that any scaled magnitude will depend only on the variable $\tilde{g} = Ng/(\hbar \omega a_{ho}^3) = 4\pi Na/a_{ho}$, where $a_{ho} = \hbar^{1/2}/(m\omega)^{1/2}$. This scaling is preserved to the extent the GP equation remains valid. For example, the $\omega$ can not be increased up to a value at which $a_{ho}$ becomes comparable to $a$.

In terms of the condensate function, the chemical potential is written as

$$\mu = \int d^3r \ \left\{ \psi^* \left( -\frac{1}{2} \Delta + \frac{1}{2} r^2 \right) \psi + \tilde{g}|\psi|^4 \right\}.$$  

It differs from the total energy per particle in half the Hartree energy

$$E = \int d^3r \ \left\{ \psi^* \left( -\frac{1}{2} \Delta + \frac{1}{2} r^2 \right) \psi + \frac{\tilde{g}}{2}|\psi|^4 \right\}$$

$$= \mu - \frac{\tilde{g}}{2} \int d^3r |\psi|^4. \quad (6)$$

We will consider formally that the variable $\tilde{g}$ ranges between zero (noninteracting bosons) and infinite (Thomas-Fermi theory). In the $\tilde{g} \rightarrow 0$ limit, we may apply perturbation theory, i.e. to look for $\psi$ and $\mu$ in the form

$$\psi = \psi_0 + \psi_1 \tilde{g} + \ldots,$$

$$\mu = \mu_0 + \mu_1 \tilde{g} + \ldots. \quad (7) \quad (8)$$

The leading contributions are given by $\psi_0 = \pi^{-3/4} e^{-r^2/2}$, $\mu_0 = 3/2$. Next corrections are easily obtained also, resulting in

$$\psi_1 = -\sum_{n>0} \frac{\langle n|\psi_0^2|0 \rangle}{2n} |n\rangle,$$

$$\mu_1 = \langle 0|\psi_0^2|0 \rangle = \frac{1}{(2\pi)^{3/2}}. \quad (9) \quad (10)$$

where the $|n\rangle$ are three-dimensional harmonic oscillator states.

The series for $E$ is obtained from (6): $E_0 = \mu_0$, whereas $E_1 = \mu_1/2$.

On the other hand, in the formal $\tilde{g} \rightarrow \infty$ limit, the kinetic energy may be neglected and the so called Thomas-Fermi (TF) theory for bosons applies. The condensate function is given by $\psi_{\infty} = \sqrt{(R^2 - r^2)/(2\tilde{R})}$, where $R = (15\tilde{g}/(4\pi))^{1/5}$, and the chemical potential reads $\mu_{\infty} = R^2/2$. The leading contribution to the energy is $E_{\infty} = 5R^2/14$.

The boundary layer near the condensate surface is responsible for the corrections to the TF theory, leading to contributions of the order of $1/R^2$.
\[ E = \frac{5}{14} R^2 + \frac{5}{2R^2} \ln(1.012 R) + \ldots \]  
(11)

\[ \mu = \frac{1}{2} R^2 + \frac{3}{2R^2} \ln(1.413 R) + \ldots \]  
(12)

Taking together the weak-coupling and strong-coupling series, for anyone of the magnitudes \( E \) and \( \mu \) we can write

\[
\begin{align*}
 f(R)|_{R \to 0} &= b_0 + b_5 R^5 + \mathcal{O}(R^{10}), \\
 |_{R \to \infty} &= R^2 \left\{ a_0 + \frac{4}{R^4} \ln(AR) + \mathcal{O}(1/R^5) \right\}.
\end{align*}
\]  
(13, 14)

The coefficients \( b_0, b_5, a_0 \) and \( a_4 \) are listed in Table 1. Notice that the variable \( R \) coincides with the condensate radius of the TF theory only in the \( \tilde{g} \to \infty \) limit (different from the notation used in Ref. [5]).

In most experimental conditions, interactions are neither so weak to be considered in perturbation theory, nor so strong for the TF theory to be valid. In the present paper, two-point Padé approximants \( \{P_{s,t}(R)\} \) are to be constructed as analytic estimates to the magnitudes \( f(R) \) over the entire range of variation of \( R \). \( s + 1 \) coefficients from the expansion (20) and \( t + 1 \) from (21) are used to determine the coefficients in the approximant. Notice that in (13-14), we have at our disposal in total 15 coefficients (many of which are equal to zero).

By construction, the approximants are asymptotically exact in both the \( R \to 0 \) and \( R \to \infty \) limits. We will show that the error of the higher approximants is lower than a few percents at any \( R \). A recent application of the Padé technique to obtain the ground-state energy of electrons in a parabolic quantum dot led to similar results.

As it is usual in Padé-approximant techniques, we shall show convergence of a sequence \( \{P_{s,t}\} \), in which both \( s \) and \( t \) increase simultaneously. In the present problem, the sequence \( \{P_{K+3,K}\} \) exhibits good convergence properties. The explicit expressions for the first nontrivial terms of this sequence are the following

\[
\begin{align*}
P_{5,2}(R) &= b_0 + b_5 R^5 + \frac{1 + q_1 R}{1 + q_1 R + q_3 R^3}, \\
q_1 &= b_0 b_5 / a_0^2, \\
q_3 &= b_5 / a_0, \\
P_{6,3}(R) &= b_0 + b_5 R^5 + \frac{1 + q_1 R}{1 + q_1 R + q_3 R^3 + q_4 R^4}, \\
q_3 &= b_5 / a_0, \\
q_1 &= 3 b_3 / (2 a_0), \\
q_4 &= b_5 q_1 / (2 a_0^2).
\end{align*}
\]  
(15-16)

We show in Fig. 1 the relative difference between \( P_{5,2} \) and \( P_{6,3} \) for the total energy per particle (the \( K = 2 \) curve). The maximum relative error of \( P_{6,3} \) may be estimated from this curve to be less than 7% over the entire range of variation of \( R \). Analogous results are obtained for the chemical potential.

To build up the next approximant, we need the \( \sim 1/R^2 \) term in the high-\( R \) series. However, this term contains a logarithmic function of \( R \). We may circumvent this problem by constructing a (7,4) interpolant for the magnitude

\[
\frac{1}{R} \frac{d}{dR} \left( R^2 f(R) \right) \bigg|_{R \to 0} = 2 b_0 + 7 b_5 R^5 + \mathcal{O}(R^{10}),
\]  
(17)

\[
|_{R \to \infty} = 4 a_0 R^2 + \frac{a_4}{R^4} + \mathcal{O}(1/R^5).\]  
(18)

The series (17-18) are similar to (13-14) up to a re-definition of coefficients: \( b_0 \rightarrow 2 b_0, \quad b_5 \rightarrow 7 b_5, \quad a_0 \rightarrow 4 a_0, \quad a_4 \rightarrow a_4 \). The approximant takes the form

\[
P_{7,4}(R) = b_0 + \frac{1}{1 + Q_1 R + Q_2 R^2 + \ldots + Q_5 R^5},
\]  
(19)

where \( Q_5 = \tilde{g} b_5 Q_2 / a_0, \quad Q_4 = \tilde{a}_0 Q_2 / b_0, \quad Q_3 = (\tilde{a}_0 / Q_2 + \tilde{b}_0) Q_5 / a_0, \quad Q_1 = Q_4 Q_5 / Q_2, \quad Q_2 \) is obtained from

\[
\tilde{a}_0 Q_1 - \tilde{b}_0 Q_3 + \tilde{a}_4 Q_5 = 0.
\]

The magnitude \( f(R) \) is obtained by multiplying by \( R \) and integrating the resulting expression. We will call it again the \( P_{7,4} \) approximant,

\[
P_{7,4}(R) = b_0 + \frac{7 b_5}{R^2} \int_0^R dx \frac{1 + Q_1 x + Q_2 x^2}{1 + Q_1 x + \ldots + Q_5 x^5}.
\]  
(20)

The integration over \( x \) could be explicitly performed, but a direct numerical integration of (20) is trivial. The coefficients \( Q_1, \ldots, Q_5 \) are listed in Table 1.

The relative difference between \( P_{7,4} \) and \( P_{6,3} \) is also shown in Fig. 1 (the \( K = 3 \) curve). The maximum error of \( P_{7,4} \) may thus be estimated to be \( \leq 1.2\% \). A similar result is obtained for \( \mu \).

Next, we turn to the two-dimensional situation. We may think of an anisotropic three-dimensional trap in which \( V_{ext} = (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) / 2 \), where \( r = \sqrt{x^2 + y^2} \), and \( \omega_z / \omega_{x,y} \gg 1 \), so that the motion of bosons in the \( z \)-direction is described by a Gaussian of very small width. Such highly anisotropic traps have been already constructed.

In eq. (1), we write \( \Psi(r,z) = \chi(z) \psi(r) \), where \( \chi(z) = (m \omega_z / (\pi \hbar))^1/4 e^{-m \omega_z z^2 / (2\hbar)} \). Multiplying the equation by \( \chi \) and integrating over \( z \), the resulting equation takes again the form (1), but the parameters entering it are \( g = g_{3D} \int dx \chi^2 = g_{3D} \sqrt{m \omega_z} / (2\pi), \mu = \mu_{3D} - h \omega_z / 2, \) and all the integrations will run over two-dimensional space. The reference level \( \mu \) for any other magnitude with dimensions of energy will be \( h \omega_z / 2 \) also.

A scaling of variables, \( r \rightarrow a_{ho} r, \quad \psi \rightarrow (N / a_{ho}^2)^{1/2} \psi, \quad \mu \rightarrow h a_{ho} \mu \), in which \( \omega = \omega_{x,y} \), reduces the GP equation to the dimensionless form (3), where \( \tilde{g} = N g / (h a_{ho}^2) \). Notice that, differently from the 3D case, \( \tilde{g} \) does not depend on \( \omega \). Thus, the dependence on \( \omega \) of any magnitude can be obtained on purely dimensional grounds. For example, any energy is exactly proportional to \( h \omega \). This is, of course, valid to the extent the GP equation is valid.
In the $\tilde{g} \to 0$ limit, the solution is looked for as (7-8), leading to

$$\psi_0 = \pi^{-1/2} e^{-r^2/2}, \quad \mu_0 = 1, \quad \text{(21)}$$

$$\psi_1 = -\sum_{n>0} \frac{\langle n|\tilde{\psi}_0^2|0\rangle}{2n}|n\rangle, \quad \text{(22)}$$

$$\mu_1 = \langle 0|\tilde{\psi}_0^2|0\rangle = \frac{1}{2\pi}. \quad \text{(23)}$$

Now, the $|n\rangle$ are two-dimensional harmonic oscillator states. The coefficients of the series for $E$ are, again, $E_0 = \mu_0$, $E_1 = \mu_1/2$.

On the other hand, in the $\tilde{g} \to \infty$ limit, TF theory leads to $\psi_\infty = \sqrt{(R^2 - r^2)/(2\tilde{g})}$, where $R = (4\tilde{g}/\pi)^{1/4}$, $\mu_\infty = R^2/2$, and $E_\infty = R^2/3$. Corrections are again given by boundary layer theory. We performed in 2D calculations similar to those of Ref. [5]. The results are

$$E = \frac{1}{3} R^2 + \frac{4}{3 R^2} \ln(1.604 R) + \ldots, \quad \text{(24)}$$

$$\mu = \frac{1}{2} R^2 + \frac{2}{3 R^2} \ln(1.435 R) + \ldots. \quad \text{(25)}$$

For anyone of the magnitudes $E$ and $\mu$, we have then

$$f(R)|_{R \to 0} = b_0 + b_4 R^4 + O(R^6), \quad \text{(26)}$$

$$|_{R \to \infty} = \frac{R^2}{2} \left\{ a_0 + \frac{a_4}{R^4} \ln(AR) + O(1/R^5) \right\}. \quad \text{(27)}$$

The coefficients are listed in Table 2.

Pade approximants are to be constructed from (26-27). Notice that, in the approximation we are working, $f(R)$ contains only even powers of $R$ or $1/R$. Thus, the maximal power in the Padé should be even. In the sequence $\{ P_{K+5,K} \}$, this leaves the approximants

$$P_{b,0}(R) = b_0 + \frac{b_4 R^4}{1 + (b_4/a_0) R^2}, \quad \text{(28)}$$

$$P_{7,2}(R) = b_0 + b_4 R^4 \frac{1 + q_2 R^2}{1 + q_2 R^2 + q_4 R^4}$$

$$q_2 = b_4 a_0/(a_0^2 - b_4), \quad q_4 = b_4 q_2/a_0. \quad \text{(29)}$$

The relative difference between $P_{b,0}$ and $P_{7,2}$ for the energy per particle in two dimensions is shown in Fig. 2 (the $K = 0$ curve). The maximum relative error of $P_{7,2}$ may be estimated to be $\leq 9\%$ ($\leq 10\%$ for $\mu$).

The next approximant in this sequence, the $P_{9,4}$, makes use not only of the $a_4$ coefficient, but of the $b_8$ as well,

$$P_{9,4}(R) = b_0 + \frac{6b_4}{R^2} \int_0^R dx \, x^5 \frac{1 + Q_2 x^2 + Q_4 x^4}{1 + Q_2 x^2 + Q_4 x^4 + Q_6 x^6}, \quad \text{(30)}$$

where $P_4 = (a_0/b_4) Q_6$, and $Q_2$, $Q_4$, $Q_6$ are obtained from the equations

$$\tilde{b}_4 Q_4 + \tilde{b}_8 = \tilde{a}_0 Q_6, \quad \text{(31)}$$

$$\tilde{a}_0 Q_4 - \tilde{b}_0 Q_6 = \tilde{b}_4 Q_2, \quad \text{(32)}$$

$$\tilde{a}_0 Q_2 - \tilde{b}_0 Q_4 = \tilde{b}_4 - \tilde{a}_4 Q_6. \quad \text{(33)}$$

The modified coefficients are $\tilde{b}_0 = 2b_0$, $\tilde{b}_4 = 6b_4$, $\tilde{b}_8 = 10b_8$, $\tilde{a}_0 = 4a_0$, $\tilde{a}_4 = a_4$. The numerical values for $Q_2$, $Q_4$, $Q_6$, and $P_3$ are listed in Table 2.

The coefficient $\tilde{b}_8$ is obtained from second order perturbation theory. For the chemical potential the result is

$$\mu_2 = 3\langle \tilde{\psi}_0^3 \rangle = \frac{3}{2} \sum_{n>0} \frac{\langle n|\tilde{\psi}_0^2|0\rangle^2}{n}. \quad \text{(34)}$$

The coefficient $E_2$ is obtained from (6), which may be rewritten in the $\tilde{g} \to 0$ limit as

$$E = \mu - \frac{\mu_1}{2} \tilde{g} - \frac{2\mu_2}{3} \tilde{g}^2 + \ldots. \quad \text{(35)}$$

The relative difference between $P_{9,4}$ and $P_{7,2}$ is drawn also in Fig. 2. It is labelled as the $K = 2$ curve. From this curve, we may estimate the maximum relative error of the $P_{9,4}$ approximant to be less than 1.8% at any $R$.

A direct comparison with the numerical calculations of Ref. [12] for the energy per particle in two dimensions in the thermodynamic ($N \to \infty$) limit is presented in Fig. 3. The difference between both results is always below the predicted 1.8%.

In conclusion, we obtained analytic Pade estimations to ground-state properties of bosons in the Gross–Pitaevskii theory. The approximants work with a small relative error ($<2\%$) at any boson density. As examples, we explicitly found the approximants for the energy per particle and the chemical potential in both three and two dimensions.

Pade approximants for other magnitudes can be constructed in the same way. Different trap geometries could be considered also. Finite systems, for which the GP formalism is no longer valid, could be studied also because we can easily apply perturbation theory near $g = 0$, and use a Hartree approximation in the $g \to \infty$ limit. Finite temperatures could be equally well considered, in particular because of the scaling of thermodynamic magnitudes. All these analytic estimations could be of great value for the experimental groups.

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M. H. Anderson, J. R. Ensher, M. R. Mathews, C. E. Wieman, and E. A. Cornell, Science 269, 198 (1995); K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, Phys. Rev. Lett. 75, 3969 (1995); C. C. Bradley, C. A. Sackett, J. J. Tollett, and R. G. Hulet, Phys. Rev. Lett. 75, 1687 (1995).

E. P. Gross, Nuovo Cimento 20, 454 (1961); L. P. Pitaevskii, Sov. Phys. - JETP 13, 451 (1961).

S. Giorgini, L. P. Pitaevskii and S. Stringari, J. Low Temp. Phys. 109, 309 (1997).

F. Dalfovo and S. Stringari, Phys. Rev. A 53, 2477 (1996).

A. L. Fetter and D. L. Feder, cond-mat/9704173.

M. J. Holland, D. S. Jin, M. L. Chiofalo, and J. Cooper, Phys. Rev. Lett. 78, 3801 (1997).

A. Gonzalez, J. Phys.: Condens. Matter 9, 4643 (1997).

A. Gonzalez, B. Partoens, and F. M. Peeters, Phys. Rev. B 56, 15740 (1997).

G. A. Baker, Jr. and P. Graves-Morris, Padé approximants (Addison-Wesley, Reading, Mass., 1981).

A. Ishihara and E. W. Montroll, Proc. Nat. Acad. Sci. 68, 3111 (1971).

M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. M. Kurn, D. S. Durfee, C. G. Townsend, and W. Ketterle, Phys. Rev. Lett. 77, 988 (1996); C. J. Myatt, E. A. Burt, R. W. Ghrist, E. A. Cornell, and C. E. Wieman, Phys. Rev. Lett. 78, 586 (1997).

T. Haugset and H. Haugerud, cond-mat/9707107.

S. Giorgini, L. P. Pitaevskii and S. Stringari, Phys. Rev. Lett 78, 3987 (1997).

FIG. 1. Relative differences between consecutive approximants for the energy in three dimensions.

FIG. 2. The same as in Fig. 1, but in two dimensions.

FIG. 3. Comparison between the $P_{3,4}$ approximant and the numerical calculations of Ref. 12 for the energy per particle in two dimensions.

|   | $E$ | $\mu$ |
|---|---|---|
| $b_0$ | 3/2 | 3/2 |
| $b_4$ | $1/(15\sqrt{2\pi})$ | $2/(15\sqrt{2\pi})$ |
| $a_0$ | 5/14 | 1/2 |
| $a_4$ | 5/2 | 3/2 |
| $Q_1$ | 0.302359 | 0.30288 |
| $Q_2$ | 0.082748 | 0.084582 |
| $Q_3$ | 0.152967 | 0.209793 |
| $Q_4$ | 0.039404 | 0.056388 |
| $Q_5$ | 0.010784 | 0.015747 |

**TABLE I. Coefficients in 3D.**

**TABLE II. Coefficients in 2D.**
\[
\frac{|P_{K+4,K+1} - P_{K+3,K}|}{P_{K+4,K+1}}
\]
\[
\frac{|P_{K+7,K+2} - P_{K+5,K}|}{P_{K+7,K+2}}
\]
Fig. 3

\[ P_{9,4}(R) \]

Ref. 12