Available online at www.sciencedirect.com
SCIENCE DIRECT®
Physica A 322 (2003) 449–455
PHYSICA A
www.elsevier.com/locate/physa

# $q$-Gaussian trial function in high density Bose–Einstein condensates

E. Erdemir, B. Tanatar*

*Department of Physics, Bilkent University, Bilkent, 06533 Ankara, Turkey*

Received 7 May 2002

**Abstract**

We study the ground-state static properties of Bose–Einstein condensates in the high density regime using a trial wave function of the form of a $q$-Gaussian. The flexibility afforded by a $q$-Gaussian trial function yields very accurate ground-state energies for large number of particles. The resulting condensate wave function profiles are also in good agreement in the high density regime. Comparing our results with those of numerical calculations we provide information on the possible limitations of the $q$-Gaussian trial functions.


*PACS:* 03.75.Fi; 05.30.Jp

Advances in the laser and evaporative cooling techniques as well as the trapping methods have culminated in successful realization of Bose–Einstein condensation in atomic gases [1]. This stirred a great deal of experimental and theoretical activity in the study of quantum gases [2]. The original experiments used dilute systems, namely when the interatomic distance is much larger than the range of interactions. More quantitatively, the dimensionless parameter $na^3 \ll 1$, where $n$ is the mean density and $a$ is the $s$-wave scattering length characterizing the interaction strength between atoms. Recently, there has been experimental [3–5] and theoretical [6–11] interest in the regime where the diluteness condition does not hold. This may be achieved either by increasing the number of atoms $N$ in the condensate, or by tuning the interaction strength (or equivalently $a$) through Feshbach resonance. Investigation of atomic systems at high density renders useful information on the role of interactions.

* Corresponding author. Tel.: +90-312-290-1591; fax: +90-312-266-4579.
*E-mail address:* tanatar@fen.bilkent.edu.tr (B. Tanatar).

0378-4371/03/$ - see front matter 
doi:10.1016/S0378-4371(02)01812-5

The ground-state static properties of dilute bosonic gases are well described by the Gross–Pitaevskii (GP) equation which assumes that all the particles are in the condensed state. Condensate density and other thermodynamic properties can be obtained by the numerical solution of the GP equation [2]. Because of their physical and intuitive content variational approaches have also been quite popular [12–14]. Recently, Fa et al. [15] introduced $q$-Gaussian trial functions to minimize variationally the GP energy functional, and have found good agreement with the results of numerical calculations. $q$-Gaussians were originally employed in the context of Tsallis' nonextensive statistics [16].

In this work we employ the $q$-Gaussian trial function as introduced by Fa et al. [15] to variationally calculate the ground-state energy and condensate wave function profiles of a Bose gas in the high density regime. We are first motivated by the success of this trial function in the low density regime and intend to test the applicability at high densities. Second, in comparing the results of the variational calculation to those of numerical methods, it was noticed [14] that some inconsistent discrepancies exist. We, thus, provide more accurate results for the numerical solution of the GP equation at high densities.

The ground state static properties of a condensed system of bosons confined in an harmonic trap and in the high density regime is described by the modified Gross–Pitaevskii (MGP) energy functional [6]. In the following, we use harmonic oscillator length $a_{\mathrm{HO}} = (\hbar/m\omega)^{1/2}$, $\hbar\omega$, and $(Na_{\mathrm{HO}}^3)^{1/2}$ to scale lengths, energies, and the condensate wave function $\psi$, respectively. In terms of the scaled variables, the MGP functional is

$$E[\psi] = \int \mathrm{d}^3 r \left[ \frac{1}{2}|\nabla\psi|^2 + \frac{1}{2}r^2|\psi|^2 + 2\pi aN|\psi|^4 \times \left(1 + \frac{128}{\sqrt{\pi}15}[Na^3|\psi|^2]^{1/2} + 8(4\pi/3 - \sqrt{3})Na^3|\psi|^2 \ln[Na^3|\psi|^2]\right)\right] . \tag{1}$$

This equation is obtained within the local-density approximation making use of the perturbatively calculated homogeneous system energy density. If the terms beyond $2\pi aN|\psi|^4$ are neglected the usual Gross–Pitaevskii (GP) energy functional is recovered. Functional minimization of the above energy subject to the normalization of $\psi$ yields the modified Gross–Pitaevskii (MGP) equation [6]

$$\left[ -\frac{1}{2}\nabla^2 + \frac{1}{2}r^2 + 4\pi aN|\psi|^2 + \frac{128}{3}\pi^{1/2}a^{5/2}N^{5/2}|\psi|^3 + 8\pi a^4N^2(4\pi/3 - \sqrt{3})|\psi|^4(6\ln(Na^3|\psi|^2) + 2)\right]\psi = \mu\psi , \tag{2}$$

where $\mu$ is the chemical potential.

Table 1
The ground-state energies per particle $E/N$ for $^{87}$Rb ($a/a_{HO} = 4.33 \times 10^{-3}$) compared in different approaches

| $N$ | $E/N$ | | | |
|---|---|---|---|---|
| | $q$-Gaussian | MTF | Numerical | Ref. [14] |
| $10^5$ | 12.24 | 12.04 | 12.19 | 12.21 |
| $10^6$ | 30.45 | 30.33 | 30.40 | 30.51 |
| $10^7$ | 76.47 | 76.41 | 76.42 | 76.75 |
| $10^8$ | 192.28 | 192.38 | 192.23 | 193.13 |
| $10^9$ | 481.55 | 482.42 | 481.55 | 483.81 |

In a previous work, Fa et al. [15] considered the $q$-Gaussian trial function to calculate the ground-state properties of an anisotropic system within the GP approximation, and found good agreement with numerical calculations. For isotropic systems, the $q$-Gaussian trial function takes the form

$$\psi(r) = \begin{cases} A[1-(1-q)\alpha r^2]^{1/(1-q)} & \text{if } 1-(1-q)\alpha r^2 > 0\,, \\ 0 & \text{otherwise}\,. \end{cases} \tag{3}$$

Here $\alpha$ and $q$ are variational parameters and $A$ is the normalization constant. As suggested by Fa et al. [15] we allow $q$ to vary from $q=1$ (which corresponds to the Gaussian wave function of an ideal gas) to $q=-1$ (which corresponds to the Thomas–Fermi limit). Similarly to the widely used Gaussian trial functions, the present $q$-Gaussians provide analytical expressions for the integrated MGP functional. [1] We have checked that $q$-Gaussian trial function within a variational approach works very well for the isotropic systems too.

We have performed variational and purely numerical calculations on a system of $^{87}$Rb atoms in an isotropic harmonic trap characterized by the angular frequency $\omega/2\pi = 77.78$ Hz. The $s$-wave scattering length for this trap frequency is given by $a = 4.33 \times 10^{-3} a_{HO}$ where $a_{HO} = (\hbar/m\omega)^{1/2}$ is the harmonic oscillator length. The numerical solution of the MGP equation is obtained by the steepest descent method [6,17]. To test the fidelity of the $q$-Gaussian trial function at high density, we consider systems with large number of particles, i.e., $N = 10^5 - 10^9$. Our variational and numerical results for the ground-state energy (per particle) $E/N$ are tabulated in Table 1, along with the variational results of Banerjee and Singh [14]. We first note that the numerical solution of the MGP equation yields ground-state energies consistently lower than the variational results for a given $N$. This is to be expected, since the variational principle ensures that the variationally calculated ground-state energy is an upper bound. Thus, the possible mistakes in the quoted numerical values of Refs. [6] and [10] are corrected. We have also checked that our $E/N$ within the MGP theory is in better agreement with the correlated basis function calculation [6]. Second,

[1] The integral of the logarithmic term can be expressed in terms of the Digamma function $\Psi(x)$. Since the analytical expressions are not particularly illuminating we omit their presentations here.

our variational results using $q$-Gaussian wave function are in better agreement with the MGP results than those of Banerjee and Singh [14] and they also satisfy the variational principle. In Table 1, we have also given the ground state energy within the Thomas–Fermi approximation for comparison. This is calculated to be [14]

$$E_{\mathrm{TF}}/N = \frac{5}{7}\,\mu_{\mathrm{TF}}\left[1 + \frac{7}{8}\,(\pi n a^3)^{1/2} + \frac{32}{15}\,(4\pi/3 - \sqrt{3})na^3 \ln\,(na^3)\right], \tag{4}$$

where the gas parameter is $na^3 = (15N)^{2/5}a^{12/5}/8\pi$. Similar levels of agreement and improvement is obtained for other quantities such as the chemical potential $\mu$, and root-mean-square of radial coordinate $\langle r^2\rangle^{1/2}$.

To elucidate the performance of the $q$-Gaussian functions within the GP and MGP approaches we have plotted the variationally determined $q$ values as a function of $N$, as shown in Fig. 1. For the GP functional without the high density corrections, $q$ has the expected dependence on $N$, which ranges from 1 (small $N$) to $-1$ (large $N$). In the case of MGP functional, $q$ shows essentially the same behavior but starts to depart from the expected $N$-dependence around $N = 10^9$. This means that the wave function profile is not very similar to the TF profile at these values of $N$. Such a behavior is not physical and it leads us to conclude that $q$-Gaussians would be less useful for $N > 10^9$. The results shown in Fig. 1(a) were calculated for the scattering length $a/a_{\mathrm{HO}} = 4.33 \times 10^{-3}$. By increasing the harmonic oscillator frequency $\omega$, or making use of the Feshbach resonance $a/a_{\mathrm{HO}}$ may be increased. We show the $N$-dependence of variational $q$ parameter for $a/a_{\mathrm{HO}} = 10^{-2}$ in Fig. 1(b). In this case, the departure from the expected behavior starts around $N = 10^6$. Using the TF result for the gas parameter, we find that for $a/a_{\mathrm{HO}} = 4.33 \times 10^{-3}$ and $N = 10^9$, one obtains $na^3 \approx 10^{-3}$. It was noted [7] that for $na^3 \gtrsim 10^{-3}$ the logarithmic term in the MGP energy functional starts to become appreciable and the validity of the perturbation expression breaks down. Thus, it is not surprising that the $q$-Gaussian trial functions also fail for $na^3 \gtrsim 10^{-3}$.

The condensate wave function $\psi(r)$ as a function of the radial distance within the present $q$-Gaussian approach is shown in Fig. 2(a) and (b). Compared to the numerical solution of the MGP equation, $q$-Gaussian wave function appears to be in very good agreement. The only discrepancy is around the edge of the condensate, because the $q$-Gaussian has a TF-like behavior.

In summary we have tested the $q$-Gaussian trial function in the regime beyond the mean-field approximation for which high density effects become noticeable. We have found that similar to the low density regime where the mean-field GP equation gives an accurate description, the variational method using $q$-Gaussian trial function also works well at higher densities. We have quantitatively calculated the regime of applicability of $q$-Gaussian trial function. We have also provided seemingly more accurate results for the ground-state properties of $^{87}$Rb gas at large particle numbers. Our calculations may straightforwardly be extended to anisotropic traps and lower dimensional systems.

This work was partially supported by the Scientific and Technical Research Council of Turkey (TUBITAK) under Grant no. TBAG-2005, by NATO under Grant no. SfP971970, by the Turkish Department of Defense under Grant no. Kobra-001, and by the Turkish Academy of Sciences.

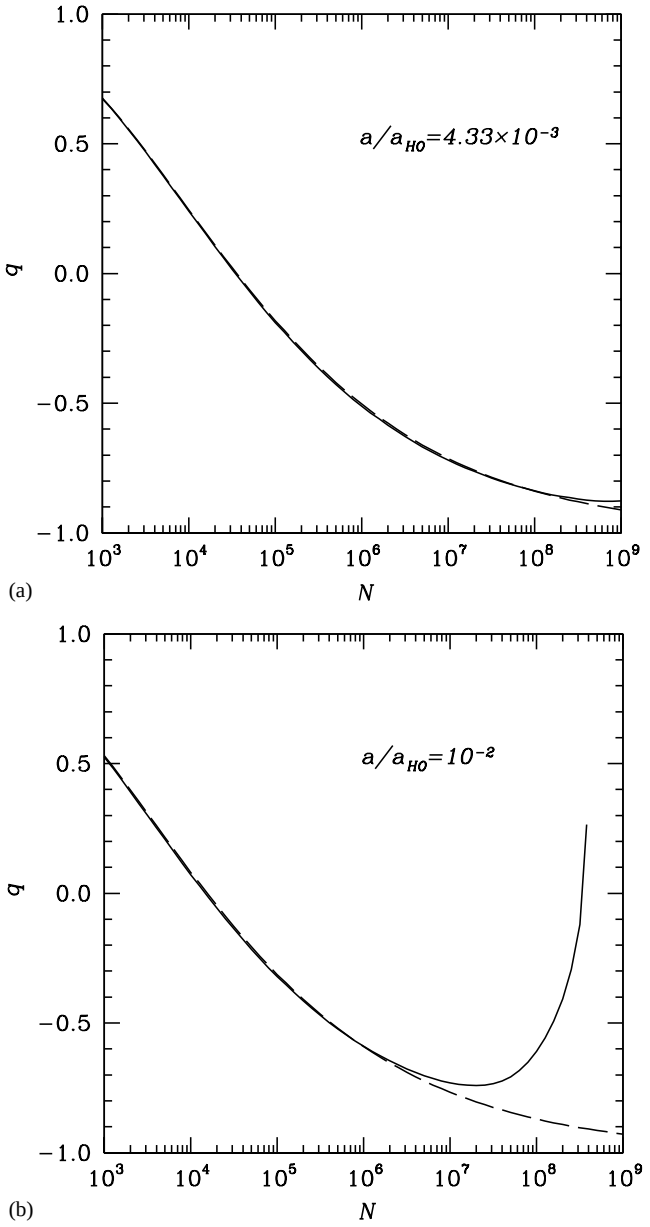


Fig. 1. The variational parameter $q$ as a function of $N$ within the GP (dashed) and MGP (solid) approaches. The interaction strength is (a) $a/a_{\mathrm{HO}} = 4.33 \times 10^{-3}$ and (b) $a/a_{\mathrm{HO}} = 10^{-2}$.

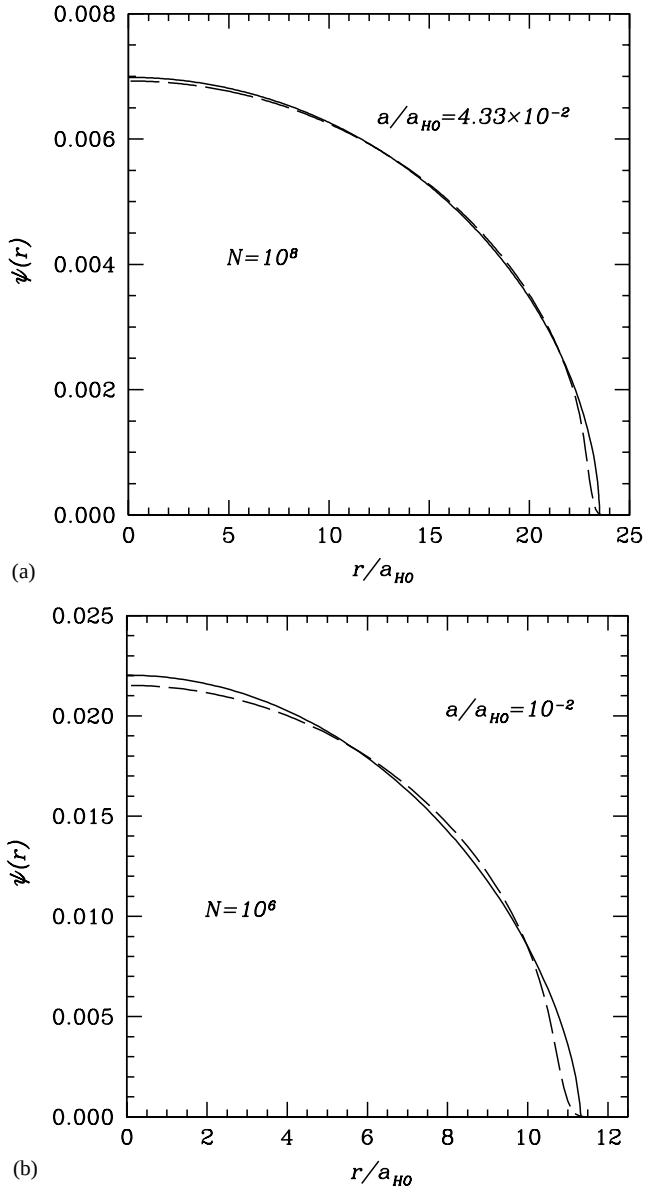


Fig. 2. The condensate wave function $\psi$ as a function of the radial distance within the $q$-Gaussian (solid lines) and numerical (dashed lines) approaches. (a) $N=10^8$, $a/a_{\mathrm{HO}}=4.33\times10^{-3}$, (b) $N=10^6, a/a_{\mathrm{HO}}=10^{-2}$.

## References

[1] M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, E.A. Cornell, Science 269 (1995) 198;
K.B. Davis, M.-O. Mewes, M.R. Andrews, N.J. van Druten, D.S. Durfee, D.M. Kurn, W. Ketterle, Phys. Rev. Lett. 75 (1995) 3969;
C.C. Bradley, C.A. Sackett, R.G. Hulet, Phys. Rev. Lett. 78 (1997) 985.
[2] F. Dalfovo, S. Giorgini, L. Pitaevskii, S. Stringari, Rev. Modern Phys. 71 (1999) 463;
A.S. Parkins, D.F. Walls, Phys. Rep. 303 (1998) 1;
V. Bagnato, D. Kleppner, Phys. Rev. A 44 (1991) 7439.
[3] N.R. Claussen, E.A. Donley, S.T. Thompson, C.E. Wieman, Phys. Rev. Lett. 89 (2002) 010401.
[4] S.L. Cornish, N.R. Claussen, J.L. Roberts, E.A. Cornell, C.E. Wieman, Phys. Rev. Lett. 85 (2000) 1795.
[5] J.L. Roberts, N.R. Claussen, S.L. Cornish, E.A. Donley, E.A. Cornell, C.E. Wieman, Phys. Rev. Lett. 86 (2001) 4211.
[6] A. Fabrocini, A. Polls, Phys. Rev. A 60 (1999) 2319.
[7] S. Giorgini, J. Boronat, J. Casulleras, Phys. Rev. A 60 (1999) 5129.
[8] A. Fabrocini, A. Polls, Phys. Rev. A 64 (2001) 063610.
[9] E. Timmermans, P. Tommasini, K. Huang, Phys. Rev. A 55 (1997) 3645.
[10] G.S. Nunes, J. Phys. B 32 (1999) 4293.
[11] E. Braaten, H.-W. Hammer, T. Mehen, Phys. Rev. Lett. 88 (2002) 040401.
[12] G. Baym, C.J. Pethick, Phys. Rev. Lett. 76 (1996) 6.
[13] A. Fetter, J. Low Temp. Phys. 106 (1997) 643.
[14] A. Banerjee, M.P. Singh, Phys. Rev. A 64 (2001) 063604.
[15] K.S. Fa, R.S. Mendes, P.R.B. Pedreira, E.K. Lenzi, Physica A 295 (2001) 242.
[16] C. Tsallis, R.S. Mendes, A.R. Plastino, Physica A 261 (1998) 534.
[17] F. Dalfovo, S. Stringari, Phys. Rev. A 53 (1996) 2477.