

Analytical trial functions for modelling a two-dimensional Bose condensate

Yu.V. Likhanova, S.B. Medvedev, M.P. Fedoruk, P.L. Chapovsky

Abstract. Approximate analytical solutions to the time-independent two-dimensional Gross–Pitaevskii equation are obtained by a variational method. The solutions found are compared with the results of direct numerical calculations. The accuracy of analytical solutions is determined under various conditions of the problem, primarily the degree of nonlinear interaction of atoms in a Bose condensate.

Keywords: Bose–Einstein condensates, two-dimensional Gross–Pitaevskii equation, variational method, trial functions, approximate analytical solutions.

1. Introduction

Many important phenomena of modern physics are described by nonlinear equations, the exact solutions of which, unfortunately, have not yet been found in a number of cases. To date, numerical methods are an effective way of solving nonlinear physics problems. However, the application of numerical methods is often very time-consuming, and the solutions obtained with their help are not universal. In this situation, approximate analytical solutions become especially useful for problems of nonlinear physics. They can be used to obtain approximate solutions of direct and inverse problems and analyse effectively experimental data. In particular, for Bose–Einstein condensates it becomes possible to recover the coefficients of the Gross–Pitaevskii equation from the experimental data, for example, the determination of the radiation-modified coefficient of the interatomic interaction in a Bose condensate [1].

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Using the variational approach, Medvedev et al. [2] developed a method for obtaining approximate analytic solutions of the two-dimensional Gross–Pitaevskii equation. The main attention was paid to the dynamic problem of the expansion of the Bose gas after switching off the magnetic trap. In the present paper, using the method proposed in [2], we obtain approximate analytical solutions of the time-independent 2D Gross–Pitaevskii equation and investigate their properties. The accuracy of the approximate analytical solutions is determined in this paper by comparing them with a direct numerical solution of the time-independent 2D Gross–Pitaevskii equation.

2. Two-dimensional Gross–Pitaevskii equation

Theoretical analysis of Bose condensates is now traditionally based on the Gross–Pitaevskii equation [3]. This equation has been especially intensively studied after the first experimental work on the creation of Bose–Einstein condensates (BECs) of rarefied gases [4, 5]. The present study has been also initiated by our paper [6], in which we compared the experimental data and numerical calculations of the expansion of the Bose condensate of rubidium atoms after switching off the magnetic trap. The three-dimensional Gross–Pitaevskii equation for the condensate wave function $\Psi(\mathbf{r}, z, \bar{t})$, $\mathbf{r} = (x, y)$ has the form [7]

$$i\hbar \frac{\partial \Psi(\mathbf{r}, z, \bar{t})}{\partial \bar{t}} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{r}, z, \bar{t}) + V(\mathbf{r}, z) \Psi(\mathbf{r}, z, \bar{t}) + NU_0 |\Psi(\mathbf{r}, z, \bar{t})|^2 \Psi(\mathbf{r}, z, \bar{t}). \quad (1)$$

Here, the wave function is normalised to unity; N is the number of condensed particles; $V(\mathbf{r}, z) = m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)/2$ is the harmonic potential of the trap; ω_x , ω_y and ω_z are the frequencies of vibrations of atoms in the trap; m is the mass of the atom; $U_0 = 4\pi\hbar^2 alm$ is the interatomic interaction; and a is the scattering length of the s -wave.

A significant simplification arises in the solution of the 2D problem. For example, for a disk-like condensate with frequencies $\omega_z \gg \omega_x \approx \omega_y$ and a chemical potential $\mu < \hbar\omega_z$, where

$$\mu \equiv \int_{\mathbb{R}^3} \left[\frac{\hbar^2}{2m} |\nabla \Psi|^2 + V(\mathbf{r}, z) |\Psi|^2 + NU_0 |\Psi|^4 \right] d\mathbf{r} dz,$$

the motion along one coordinate turns out to be ‘frozen’. In this case, the condensate wave function can be written in the form [7]

$$\Psi(r, z, \bar{t}) = \Psi_r(r, \bar{t}) \frac{1}{\pi^{1/4} l_z^{1/2}} \exp(-z^2/2l_z^2),$$

$$l_z = \sqrt{\hbar/m\omega_z},$$

and $\Psi_r(r, \bar{t})$ is found as the solution of the 2D Gross–Pitaevskii equation

$$\begin{aligned} i\hbar \frac{\partial \Psi_r(r, \bar{t})}{\partial \bar{t}} = & -\frac{\hbar^2}{2m} \nabla_r^2 \Psi_r(r, \bar{t}) + V(r) \Psi_r(r, \bar{t}) \\ & + \frac{NU_0}{\sqrt{2\pi} l_z} |\Psi_r(r, \bar{t})|^2 \Psi_r(r, \bar{t}), \end{aligned} \quad (2)$$

where $V(r) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2)$, with the normalisation

$$\int_{\mathbb{R}^2} |\Psi_r(r, \bar{t})|^2 dr = 1.$$

In this paper we confine ourselves to an analysis of 2D Bose condensates, which are described by Eqn (2). For convenience, we will consider the 2D Gross–Pitaevskii equation in a dimensionless form,

$$\begin{aligned} i \frac{\partial \psi(x, t)}{\partial t} = & -\frac{s}{2} \nabla^2 \psi(x, t) + V(x) \psi(x, t) \\ & + \sigma |\psi(x, t)|^2 \psi(x, t), \end{aligned} \quad (3)$$

where $V(x) = \frac{1}{2}(a_1^2 x_1^2 + a_2^2 x_2^2)$, with the normalisation

$$\mathcal{N} = \int_{\mathbb{R}^2} |\psi(x, t)|^2 dx = 1. \quad (4)$$

For equation (2) to be reduced to equation (3) in dimensionless variables, it is necessary to replace $\bar{t} = t\omega_x/\sqrt{s}$, $r = x/r_s$ and $\Psi_r(r, \bar{t}) = r_s \psi(x, t)$; in this case, the coefficients of the equations are related to each other in the following way:

$$\begin{aligned} a_1 = 1, \quad a_2 = \omega_y/\omega_x, \quad s = (l_x/r_s)^4, \quad \sigma = \delta s^{5/4}, \\ \delta = 2\sqrt{2\pi} aN/(l_x l_z), \quad l_x = \sqrt{\hbar/(m\omega_x)}, \quad l_z = \sqrt{\hbar/(m\omega_z)}, \end{aligned} \quad (5)$$

where r_s is the characteristic size of the condensate [in the case of a weakly interacting condensate, we can take $r_s = O(l_x)$].

3. Variational solution of the problem

Equation (3) can be obtained from the standard action (for details, see [2])

$$S = \int_{-\infty}^{\infty} \left[\int_{\mathbb{R}^2} \left(\frac{i}{2} \bar{\psi} \frac{\partial \psi}{\partial t} - \frac{i}{2} \psi \frac{\partial \bar{\psi}}{\partial t} \right) dx - \mathcal{H} \right] dt \quad (6)$$

with the Hamiltonian

$$\mathcal{H} = \int_{\mathbb{R}^2} \left[\frac{s}{2} |\nabla \psi|^2 + V |\psi|^2 + \frac{\sigma}{2} |\psi|^4 \right] dx. \quad (7)$$

We introduce the representation

$$\psi(x, t) = B(x, t) \exp(i\varphi(x, t)), \quad (8)$$

where $B(x, t)$ and $\varphi(x, t)$ are real functions. It can be shown that \mathcal{H} contains even powers: $B^2(x, t)$ and $B^4(x, t)$. The

potential $V(x)$ is symmetric with respect to reflections from the coordinate axes, and therefore the functions φ and B^2 are also symmetric. For the phase φ we confine ourselves to the first terms of the expansion in the Maclaurin series,

$$\varphi(x, t) = \varphi_0 + \varphi_1 x_1^2 + \varphi_2 x_2^2, \quad (9)$$

and we represent the function B^2 in the form

$$B^2(x_1, x_2, t) = Af(B_1 x_1, B_2 x_2). \quad (10)$$

Here, $\varphi_0, \varphi_1, \varphi_2, A, B_1$ and B_2 are the time-independent functions; and $f(\xi)$ [$\xi = (\xi_1, \xi_2)$] is some symmetric trial function normalised so that the zero moment and the second moments are equal to unity:

$$\int_{\mathbb{R}^2} \xi f(\xi) d\xi = 0, \quad \int_{\mathbb{R}^2} f(\xi) d\xi = 1, \quad \int_{\mathbb{R}^2} \xi_i^2 f(\xi) d\xi = 1.$$

Examples of specific trial functions $f(\xi)$ are considered in Section 4.1.

Representations (9) and (10) make it possible to replace the action of \mathcal{S} (6) for equation (3) by its finite-dimensional approximation

$$S = - \int_{-\infty}^{\infty} \left(Q_0 \frac{dP_0}{dt} + Q_1 \frac{dP_1}{dt} + Q_2 \frac{dP_2}{dt} + H \right) dt, \quad (11)$$

where the Hamiltonian has the form

$$\begin{aligned} H = & \frac{s}{2}(P_1^2 + P_2^2) + \frac{sQ_0^2}{2} \left(\frac{C_1}{Q_1^2} + \frac{C_2}{Q_2^2} \right) \\ & + \frac{1}{2}(a_1^2 Q_1^2 + a_2^2 Q_2^2) + \frac{\sigma Q_0^3}{2} \frac{C_0}{Q_1 Q_2}. \end{aligned} \quad (12)$$

Here, the constants C_0, C_1 and C_2 are defined in terms of the integrals of the function $f(\xi)$:

$$C_0 = \int_{\mathbb{R}^2} f^2 d\xi_1 d\xi_2, \quad C_i = \int_{\mathbb{R}^2} \left(\frac{\partial f^{1/2}}{\partial \xi_i} \right)^2 d\xi_1 d\xi_2, \quad i = 1, 2. \quad (13)$$

The parameters P_1, P_2, Q_1 and Q_2 are related to the functions $B(x, t)$ and $\varphi(x, t)$ as follows:

$$A = \frac{Q_0^2}{Q_1 Q_2}, \quad B_1 = \frac{Q_0^{1/2}}{Q_1}, \quad B_2 = \frac{Q_0^{1/2}}{Q_2}, \quad (14)$$

$$\varphi_1 = \frac{P_1}{2Q_1}, \quad \varphi_2 = \frac{P_2}{2Q_2},$$

where Q_0 is the zero moment; and Q_1 and Q_2 are the corresponding characteristic dimensions of the function B^2 .

The Hamiltonian H does not depend on P_0 ; therefore, Q_0 is an integral of the finite-dimensional system given by (11) and coincides with the integral of the original continuous system (3). In accordance with the normalisation (4), $Q_0 = \mathcal{N} = 1$. Equation (3) can be reduced to finite-dimensional equations of motion [2]

$$\frac{dP_1}{dt} = -a_1^2 Q_1 + \frac{sC_1}{Q_1^3} + \frac{\sigma}{2} \frac{C_0}{Q_1^2 Q_2}, \quad \frac{dQ_1}{dt} = sP_1, \quad (15)$$

$$\frac{dP_2}{dt} = -a_2^2 Q_2 + \frac{sC_2}{Q_2^3} + \frac{\sigma}{2} \frac{C_0}{Q_1 Q_2^2}, \quad \frac{dQ_2}{dt} = sP_2, \quad (16)$$

which are obtained by varying the finite-dimensional action (11).

Thus, the problem of finding the solution of (8) reduces to determining the quantities Q_1 , Q_2 , P_1 and P_2 from the given parameters of the problem, a_1 , a_2 , s and σ . The parameters C_0 , C_1 and C_2 are given by the form of the normalised trial function $f(\xi)$ by formula (13).

To find the time-independent solution of the Hamiltonian system (11), (12), it is sufficient to equate to zero the time derivatives in equations of motion (15), (16). This gives $P_1 = P_2 = 0$ and a system of algebraic equations for Q_1 and Q_2 :

$$-a_1^2 Q_1 + \frac{sC_1}{Q_1^3} + \frac{\sigma}{2} \frac{C_0}{Q_1 Q_2} = 0, \quad (17)$$

$$-a_2^2 Q_2 + \frac{sC_2}{Q_2^3} + \frac{\sigma}{2} \frac{C_0}{Q_1 Q_2} = 0. \quad (18)$$

The numerical solution of these equations gives stationary values of Q_1 , Q_2 , substitution of which in the chosen trial function (10) gives the required time-independent solution (see Section 4.2):

$$B^2(x_1, x_2) = f\left(\frac{1}{Q_1} x_1, \frac{1}{Q_2} x_2\right) \frac{1}{Q_1 Q_2}. \quad (19)$$

The steady-state value of the chemical potential μ is found from the equation

$$\mu = -\frac{dP_0}{dt} = \frac{\partial H}{\partial Q_0} = sQ_0 \left(\frac{C_1}{Q_1^4} + \frac{C_2}{Q_2^4} \right) + \frac{3}{2} \sigma C_0 \frac{Q_0^2}{Q_1 Q_2}.$$

If we set trap parameters a_1 , a_2 and condensate sizes Q_1 , Q_2 , then the parameters s and σ can be found from formulas

$$s = \frac{Q_1^2 Q_2^2 (a_2^2 Q_2^2 - a_1^2 Q_1^2)}{C_2 Q_1^2 - C_1 Q_2^2}, \quad (20)$$

$$\sigma = 2 \frac{Q_1 Q_2 (C_2 a_1^2 Q_1^4 - C_1 a_2^2 Q_2^4)}{C_0 (C_2 Q_1^2 - C_1 Q_2^2)}.$$

Since we only consider the positive values of s and σ , not all combinations of the initial parameters correspond to this condition. There are two mutually exclusive situations for which s and σ are positive:

$$\frac{a_1^2}{a_2^2} \leq \frac{Q_2^2}{Q_1^2} \leq \sqrt{\frac{C_2}{C_1}} \frac{a_1}{a_2}, \quad \sqrt{\frac{C_2}{C_1}} \frac{a_1}{a_2} \leq \frac{Q_2^2}{Q_1^2} \leq \frac{a_1^2}{a_2^2}. \quad (21)$$

Below, we will assume that $a_2 \sqrt{C_2} \geq a_1 \sqrt{C_1}$, and consider the first condition from (21), which imposes a restriction on the ratio of the sizes.

We use Hamiltonian (12) of the variational formulation of the problem and introduce the notation for its linear (l), potential (v) and nonlinear (n) parts:

$$l = \frac{s}{2} \left(\frac{C_1}{Q_1^2} + \frac{C_2}{Q_2^2} \right), \quad v = \frac{1}{2} (a_1^2 Q_1^2 + a_2^2 Q_2^2), \quad n = \frac{\sigma C_0}{2} \frac{1}{Q_1 Q_2}.$$

Substituting the values of s and σ into l , n and H , we obtain

$$l = \frac{(a_2^2 Q_2^2 - a_1^2 Q_1^2)(C_2 Q_1^2 + C_1 Q_2^2)}{2(C_2 Q_1^2 - C_1 Q_2^2)},$$

$$n = \frac{C_2 a_1^2 Q_1^4 - C_1 a_2^2 Q_2^4}{C_2 Q_1^2 - C_1 Q_2^2}, \quad (22)$$

$$H = l + v + n = 2v = a_1^2 Q_1^2 + a_2^2 Q_2^2.$$

The expression for the Hamiltonian follows from the virial relation $l + n = v$, which can be verified directly. Moreover, the coefficients C_0 , C_1 and C_2 can be any positive numbers. It is interesting that the value of H formally depends on a_1 , a_2 and Q_1 , Q_2 and does not depend on the values of s and σ or C_0 , C_1 and C_2 .

We introduce the parameter ν for the ratio of the linear and the nonlinear parts of the Hamiltonian:

$$\nu = \frac{l}{n} = \frac{(a_2^2 Q_2^2 - a_1^2 Q_1^2)(C_2 Q_1^2 + C_1 Q_2^2)}{2(C_2 a_1^2 Q_1^4 - C_1 a_2^2 Q_2^4)}. \quad (23)$$

This formula allows us to determine the single-valued positive Q_2 from positive parameters a_1 , a_2 and from the positive nonlinearity level ν and the value of Q_1 . Then, using formula (20), we can find s and σ . Here the coefficients C_0 and C_1 are determined from the form of the normalised trial function by formula (13). Thus, using the nonlinearity parameter, it is convenient to specify various nonlinear regimes for the given parameters of the trap and the size of the condensate. The magnitude of the nonlinearity dictates the choice of the trial function. For the average nonlinearity $\nu = 1$, as a trial function, we select a Gaussian function with the corresponding values of C_0 and C_1 . For the strongly nonlinear case, when the Thomas–Fermi approximation is valid, we take the super-Gaussian function as a trial function.

4. Trial functions

As analytical trial functions, we consider the Gaussian function, the Thomas–Fermi function of the Gross–Pitaevskii equation with a harmonic potential and the super-Gaussian function [8].

4.1. Normalised trial functions

The normalised Gaussian variational function has the form

$$f_{vG}(\xi) = \frac{1}{2\pi} \exp\left(-\frac{\xi^2}{2}\right),$$

where $\xi = \sqrt{\xi_1^2 + \xi_2^2}$. The constants C_0 and C_1 are as follows:

$$C_0 = \frac{1}{4\pi}, \quad C_1 = C_2 = \frac{1}{4}. \quad (24)$$

This function is most common in the variational method, since it allows one to calculate the majority of integrals explicitly.

The Thomas–Fermi solution is widely used to describe BECs. In the normalised form this solution has the form

$$f_{\text{TF}}(\xi) = \frac{6 - \xi^2}{18\pi}. \quad (25)$$

Since the terms with the Laplacian are neglected in this approximation, in further calculations we can set $C_1 = C_2 = 0$. Thus, for the calculations we have

$$C_0 = \frac{2}{9\pi}, \quad C_1 = C_2 = 0. \quad (26)$$

In the case of strong nonlinearity, the Thomas–Fermi approximation works well, but has singularities. Therefore, it was suggested in [9] to use smooth approximations obtained by expanding the exponent for the exponential representation of the Thomas–Fermi function.

We consider a super-Gaussian function, which is smooth. The choice of the free parameter k makes it possible to approximate it sufficiently well to the Thomas–Fermi function from the condition that the values of the normalised Thomas–Fermi and super-Gaussian functions at a zero level coincide. The normalised super-Gaussian function has the form:

$$f_{\text{sG}}^k(\xi) = \frac{1}{4\pi} \frac{\Gamma(4k+1)}{\Gamma^2(2k+1)} \exp\left[-\left(\frac{\xi}{2} \sqrt{\frac{\Gamma(4k+1)}{\Gamma(2k+1)}}\right)^{1/k}\right],$$

where Γ is the gamma function; and the parameter $k > 0$. For $k = 1/2$ we obtain the normalised Gaussian function. The corresponding constants are as follows:

$$C_0 = \frac{4^{k-1}\Gamma(2k+1/2)}{\pi^{3/2}\Gamma(2k+1)}, \quad C_1 = C_2 = \frac{16^{k-1}\Gamma(2k+1/2)}{\sqrt{\pi}k\Gamma(2k+1)}.$$

We numerically find the value $k_* = 0.2791$ from the condition

$$f_{\text{sG}}^{k_*}(0) = f_{\text{TF}}(0) \quad \text{or} \quad \frac{1}{3\pi} = \frac{1}{4\pi} \frac{\Gamma(4k_*+1)}{\Gamma^2(2k_*+1)},$$

to which there correspond the constants

$$C_0 = 0.0721, \quad C_1 = 0.2986. \quad (27)$$

Note also that the parameter k can be chosen from other criteria for the closeness of the super-Gaussian function and the Thomas–Fermi function. For example, we can choose a value of k so that the fourth moments of the solution of these two functions coincide. In this case, for probabilistic distributions, their excess is said to be the same. For the Gauss function, the excess is zero.

4.2. Approximate analytical solutions

In Section 4.1 the trial functions were presented in the normalised form. Here we give approximate analytic solutions obtained with the help of these normalised functions. Taking into account formula (19) and formulas for the normalised trial functions, we obtain the approximations:

Gaussian variation function:

$$\phi_{\text{vG}}(x_1, x_2) = \frac{1}{\sqrt{2\pi}Q_1Q_2} \exp\left(-\frac{x_1^2}{4Q_1^2} - \frac{x_2^2}{4Q_2^2}\right); \quad (28)$$

super-Gaussian function:

$$\phi_{\text{sG}}(x_1, x_2) = \sqrt{f_{\text{sG}}(x_1, x_2)}, \quad (29)$$

where

$$f_{\text{sG}}(x_1, x_2) = \frac{1}{4\pi Q_1 Q_2} \frac{\Gamma(4k+1)}{\Gamma^2(2k+1)} \times \exp\left\{-\left[\frac{1}{2} \sqrt{\left(\frac{x_1^2}{Q_1^2} + \frac{x_2^2}{Q_2^2}\right) \frac{\Gamma(4k+1)}{\Gamma(2k+1)}}\right]^{1/k}\right\},$$

$$k^* = 0.2791;$$

Thomas–Fermi approximation:

$$\phi_{\text{TF}}(x_1, x_2) = \frac{1}{3\sqrt{2\pi}Q_1Q_2} \sqrt{6 - \left(\frac{x_1^2}{Q_1^2} + \frac{x_2^2}{Q_2^2}\right)}. \quad (30)$$

A direct verification shows that the variational method yields exactly the same result as the standard Thomas–Fermi approximation:

$$\phi(x_1, x_2) = \begin{cases} \sqrt{\frac{\mu - V(\mathbf{x})}{\sigma}}, & V(\mathbf{x}) < \mu, \\ 0, & V(\mathbf{x}) \geq \mu, \end{cases}$$

where $\mu = \sqrt{\sigma a_1 a_2 / \pi}$ is found from normalisation (4).

We note that the quantities Q_1 and Q_2 from the variational solution coincide in this case with the prescribed sizes of the cloud:

$$Q_1 = \sigma_1 = \sqrt{\langle (x_1 - \langle x_1 \rangle)^2 \rangle}, \quad Q_2 = \sigma_2 = \sqrt{\langle (x_2 - \langle x_2 \rangle)^2 \rangle},$$

where

$$\langle f(\mathbf{x}) \rangle \equiv \int_{\mathbb{R}^2} f(\mathbf{x}) |\psi(\mathbf{x}, t)|^2 d\mathbf{x}.$$

5. Comparison of analytical and numerical solutions

To find the stationary solution $\psi_{\text{st}}(\mathbf{x}) = \phi(\mathbf{x})$ of equation (3) corresponding to the minimum energy level, we used the imaginary-time method [10] and iterative refinement to stabilise the solution [11].

In this section we compare the results obtained with the help of numerical and variational methods for a weakly anisotropic trap. It is shown how variational approximations behave. In addition, we have compared the numerical solution and the solution obtained using the Gaussian function, which is an analytical solution of the corresponding linear problem [in the equation (3), the coefficient $\sigma = 0$]

$$\phi_{\text{G}}(x_1, x_2) = \frac{\sqrt[4]{a_1 a_2}}{\sqrt{\pi} \sqrt[4]{s}} \exp\left(-\frac{a_1 x_1^2 + a_2 x_2^2}{2\sqrt{s}}\right), \quad (31)$$

because this function is often used to evaluate the solution in practice.

Numerical experiments are constructed in terms of the integral level of nonlinearity $[v]_{\text{vG}} = [l/n]_{\text{vG}}$ [see formula (23)]. This approach allows us to more correctly and clearly determine the type of the equation (strongly, weakly or medium-

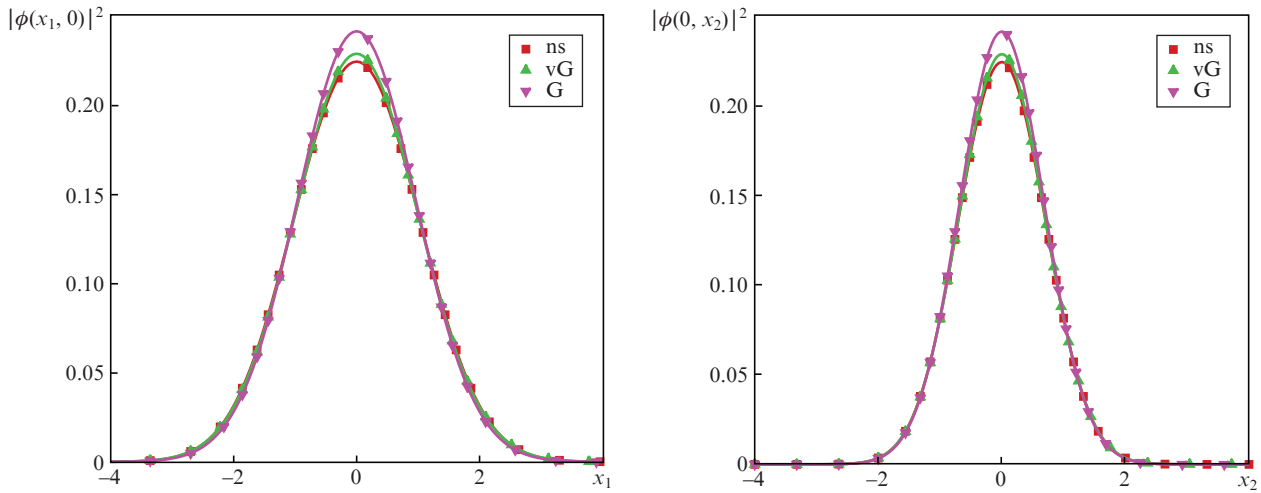


Figure 1. (Colour online) Density profiles of the solution in the case of weak nonlinearity: $[l/n]_{vG} = 10$ ($[l/n]_{ns} = 10.078$).

linear) and to show the possibilities of using the variational method.

In all numerical experiments, the trap potential parameters are $a_1 = 1, a_2 = 2$. The problem was solved in the domain $S^2 = [-6.6] \times [-4.4]$.

The results of direct numerical simulation are compared with the approximate analytical solutions presented above: the Gaussian variational function $\phi_{vG}(x_1, x_2)$ (28); super-Gaussian function $\phi_{sG}(x_1, x_2)$ (29); the Thomas–Fermi function $\phi_{TF}(x_1, x_2)$ and the Gaussian function, which is the exact solution of the linear problem, $\phi_G(x_1, x_2)$ (31).

The behaviour of the density profiles of the solution $|\psi_{st}(x_1, x_2)|^2 = |\phi(x_1, x_2)|^2$ is shown in Figs 1–3.

Figures 4 and 5 show dependences of relative errors of various integral characteristics (sizes Q_1, Q_2 , Hamiltonian \mathcal{H} and chemical potential μ of the system) on the nonlinearity parameter $v_{vG} = [l/n]_{vG}$ in the case of different solutions. The relative error was calculated as follows. For example, for the variational Gaussian function, the value of err_{Q_1} was found from the formula

$$err_{Q_1}^{vG} = \frac{|Q_1^{vG} - Q_1^{ns}|}{\max(Q_1^{vG}, Q_1^{ns})} \times 100\%,$$

where the superscript ‘ns’ corresponds to a numerical solution. For other types of functions, the relative error was calculated in a similar way.

The results of the comparison of the variational approach and direct numerical simulation presented in this section can be used as follows. From the coefficients of equation (3) we find the values of the parameters Q_1, Q_2 and then determine the level of nonlinearity in terms of the Gaussian variational function $(v)_{vG} = [l/n]_{vG}$. This value makes it possible to choose the appropriate trial function (based on the comparison results presented: in weakly nonlinear and medium-linear cases, the variational Gaussian function; in the strongly nonlinear case, the super-Gaussian function or the Thomas–Fermi approximation) and to construct the variational approximation. Then, we use it for preliminary estimation of the solution, setting the initial approximation for the iterative process or for estimating the integral parameters [which, as we see

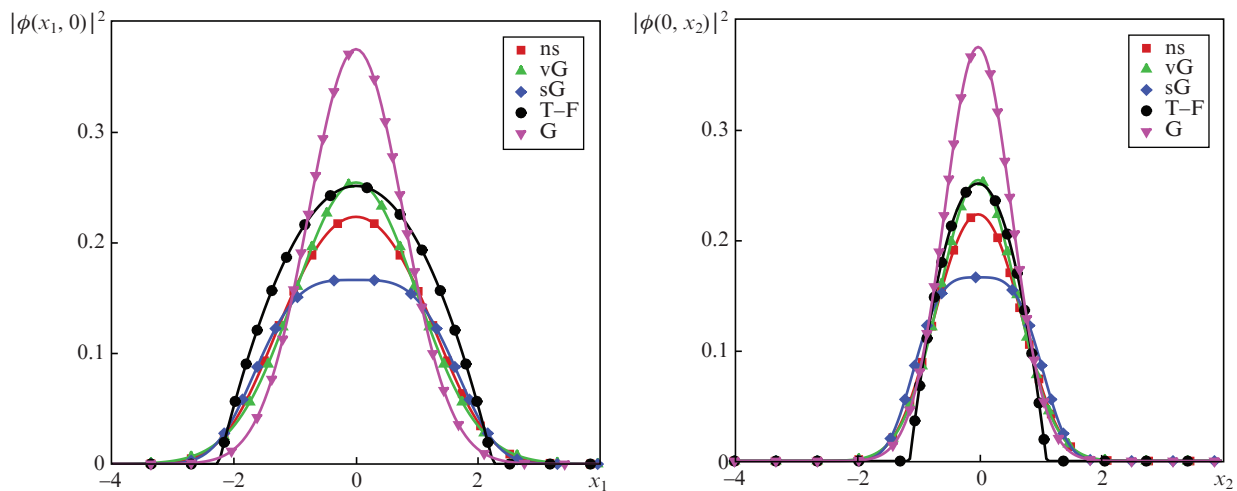


Figure 2. (Colour online) Density profiles of the solution in the case of average strong nonlinearity: $[l/n]_{vG} = 1$ ($[l/n]_{ns} = 1.067$).

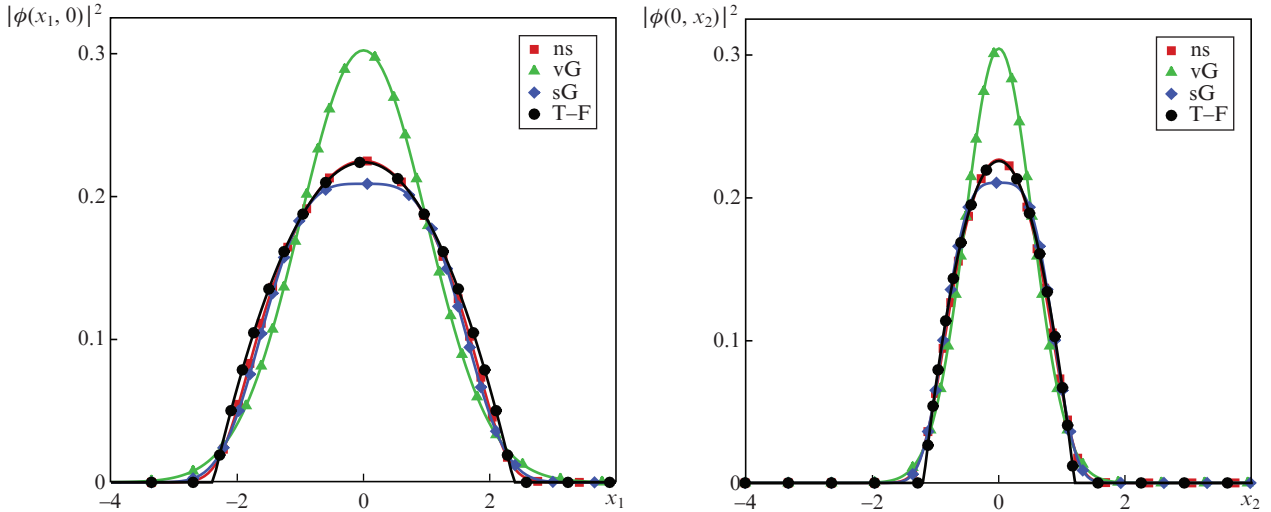


Figure 3. (Colour online) Profiles and densities in the case of strong nonlinearity: $[ln]_{vG} = 0.1$ ($[ln]_{ns} = 0.13$).

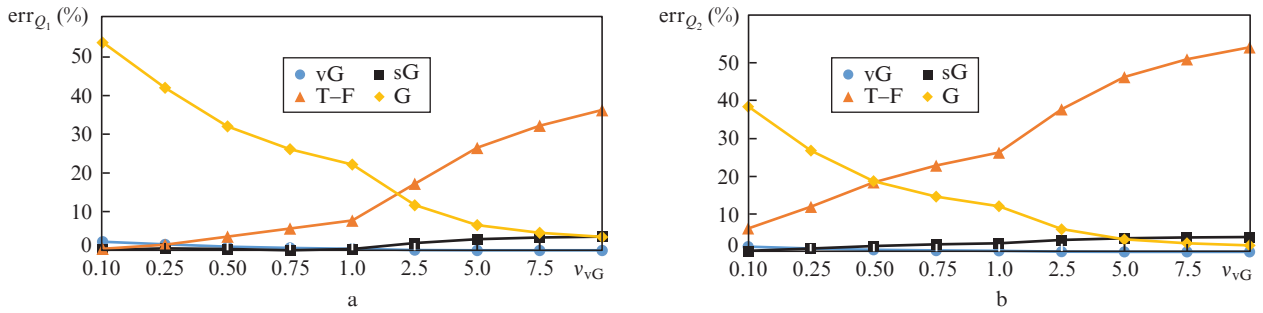


Figure 4. (Colour online) Dependences of the relative error in the sizes (a) err_{Q_1} and (b) err_{Q_2} on the nonlinearity parameters $(v)_{vG} = [ln]_{vG}$.

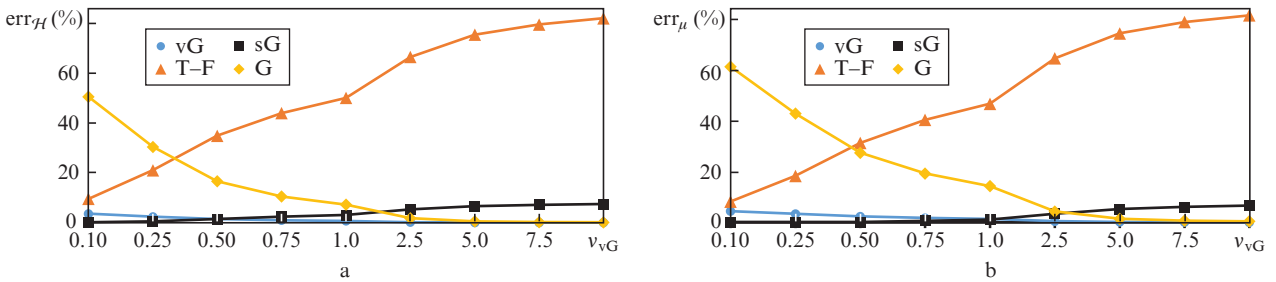


Figure 5. (Colour online) Dependences of the relative error of (a) the Hamiltonian err_H and (b) the chemical potential err_μ on the nonlinearity parameters $(v)_{vG} = [ln]_{vG}$.

from numerical experiments (Figs 4,5), are approximated with a high accuracy by the variational approach].

Note also the significant role of anisotropy, which manifests itself in the dependence of the shift of the applicability domain of trial functions on the longitudinal and transverse sizes of the trap. For Q_1 , the intersection points of the error curves for trial functions fall to a lower level of nonlinearity (for a larger inverse nonlinearity) compared to the corresponding points for Q_2 .

In addition, the proposed approach can also be used to evaluate information about the problem. For example, using formula (20), the values of the coefficients s, σ , directly related to the number of particles and the interatomic interaction [see

formula (5)] can be reconstructed from the prescribed condensate sizes Q_1, Q_2 and the trap parameters a_1, a_2 .

6. Conclusions

We have obtained approximate analytical solutions and formulas relating the integral characteristics of stationary Bose condensates (characteristic scales, Hamiltonian and chemical potential, number of particles) with the parameters of the equation (oscillation frequency of atoms in the trap, nonlinearity parameter). These analytical relations allow one to solve both the direct problem of determining the characteristics of the Bose condensate with respect to the parameters of

the Gross–Pitaevskii equation and the inverse problem of reconstructing the parameters of the equation with respect to certain given characteristics of the problem, for example, from the given size of the cloud.

The presented method is heuristic, and therefore the accuracy of the found approximate analytical functions (Gaussian, super-Gaussian and Thomas–Fermi solution) is verified by comparison with the numerical solution of the 2D Gross–Pitaevskii equation. A comparison has been made for various levels of nonlinearity and has shown that the use of the solution of the linearised equation and the Thomas–Fermi solution is limited by the weak and very strong nonlinearities, respectively. At the same time, for the intermediate values of the nonlinearity parameter, the variational approach based on the Gaussian and super-Gaussian functions demonstrates greater accuracy. In addition, for the values of the nonlinearity parameter considered above, the super-Gaussian function with a fixed degree is more accurate than the Thomas–Fermi solution. For trial functions, the anisotropy has a significant influence on the comparative accuracy. The Thomas–Fermi approximation becomes better than the linear approximation at a greater level of nonlinearity and a smaller transverse size.

Note also that we can choose other trial functions, except for those proposed in this paper, for example exponential approximations for the Thomas–Fermi solution [9]. In the first order, this approximation coincides with the Gaussian function, while in the higher order it is very close to the Thomas–Fermi solution at the zero point. In addition, rational functions with a compact carrier can also be used [12], although they, like the Thomas–Fermi solution, have singularities.

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