Solutions of the Gross-Pitaevskii equation in two dimensions

M D Lee† and S A Morgan‡
† Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford OX1 3PU, U.K.
‡ Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, U.K.

Abstract. In two dimensions the Gross-Pitaevskii equation for a cold, dilute gas of bosons has an energy dependent coupling parameter describing particle interactions. We present numerical solutions of this equation for bosons in harmonic traps and show that the results can be quite sensitive to the precise form of the coupling parameter that is used.

PACS numbers: 03.65.Nk, 03.75.Fi
1. Introduction

The experimental realization of Bose-Einstein condensation (BEC) in dilute atomic gases has prompted a great deal of work on the theoretical description of such systems. Underlying many theoretical treatments is the notion that the condensate behaviour is governed, to first order, by the Gross-Pitaevskii equation (GPE). Recent experiments [1] and proposals [2, 3, 4] for BEC in two dimensional (2D) traps have triggered interest in the properties of condensates in 2D. Although long wavelength fluctuations prohibit BEC in a 2D homogeneous system at any finite temperature [5], the presence of a trapping potential alters the density of states sufficiently that finite temperature 2D Bose condensates may be created in trapped systems [6]. Such condensates obey a modified form of the Gross-Pitaevskii equation, which contains the correct description of scattering in 2D. In a recent paper [7] we derived this description based on an approximation of the many-body T-matrix in terms of the off-shell two-body T-matrix. In this paper we present numerical solutions of the 2D GPE for ground state and vortex states of a zero temperature gas of bosons in a harmonic trap, and contrast the results with other forms that have been suggested recently [8]. We show that the detailed numerical predictions are quite sensitive to the precise form of the interaction strength used.

In the following section we summarize the scattering theory needed to describe interactions in a 2D homogeneous BEC, before discussing in section 3 the various approximations by which these results may be applied to a trapped gas. Finally, in section 4 we present numerical results for each of these approximations and discuss the significant differences which can arise between them.

2. The Gross-Pitaevskii equation and scattering

The condensate wave function $\psi(r)$ is given by the solution of the two dimensional Gross-Pitaevskii equation

$$\frac{-\hbar^2}{2m} \nabla^2 \psi(r) + V_{\text{trap}}(r) \psi(r) + N_0 g_{2D}(r) |\psi(r)|^2 \psi(r) = \mu \psi(r),$$

(1)

where $V_{\text{trap}}(r)$ is an external trapping potential (which is generally harmonic in present BEC experiments), $N_0$ is the condensate population, and $\mu$ is the chemical potential. The coupling parameter $g_{2D}(r)$ appearing in the non-linear term describes the interactions between two condensate atoms.

A collision between two atoms in momentum states $|k\rangle$ and $|m\rangle$ which produces a transition to states $|i\rangle$ and $|j\rangle$ is described by the T-matrix element $\langle ij | T(E) | km \rangle$, where $E$ is the energy of the collision. The T-matrix is obtained as the solution of a Lippmann-Schwinger equation or equivalently via a summation of ladder diagrams [9]. In three-dimensional (3D) systems the coupling parameter in the GPE is often taken to be the zero-energy, zero-momentum limit of the two-body T-matrix, which describes the scattering of particles in a vacuum. This gives $\langle 00 | T_{2b}(0) | 00 \rangle = g_{3D} = 4\pi\hbar^2a_{3D}/m$ where $a_{3D}$ is the s-wave scattering length [4]. This is, however, merely an approximate description since the scattering of two condensate particles actually occurs in a medium consisting of the surrounding particles rather than in a vacuum. Instead the collision is properly described by a many-body T-matrix element $\langle 00 | T_{MB}(0) | 00 \rangle$ which incorporates the effects of the surrounding atoms on the scattering process. In 3D the many-body T-matrix leads to a relatively small correction to the two-body
T-matrix approximation (of relative order \((na_{3D}^2)^{1/2}\) at \(T = 0\)) and for many purposes it is sufficient to neglect many-body effects in the GPE. In two dimensions (and lower), however, the two-body T-matrix vanishes in the zero-energy, zero-momentum limit \([10]\), and many-body effects are therefore of much greater importance and contribute even at leading order.

In a recent paper \([7]\) we demonstrated how the many-body T-matrix can be approximated by the two-body T-matrix evaluated off the energy shell. The coupling constant which appears in the GPE in a homogeneous 2D system was shown to be

\[
g_{2D} = \langle 00| T_{\text{MB}}(0)|00\rangle = \langle 00| T_{2b}(-\mu)|00\rangle.
\]

Using the expression for the off-shell two-body T-matrix found in reference \([10]\), gives the following form of the coupling parameter in a homogeneous system \([7]\)

\[
g_{2D} = \frac{4\pi \hbar^2}{m} \frac{1}{\ln \left(\mu ma_{2D}^2/4\hbar^2\right)},
\]

where \(a_{2D}\) is a two-dimensional scattering length. For a 2D gas of hard spheres of radius \(a\) we have \(a_{2D} = ae^{\gamma_{\text{EM}}}\), where \(\gamma_{\text{EM}} \approx 0.577\) is the Euler-Mascheroni constant which we have absorbed into the definition of \(a_{2D}\) here for convenience. In practice, a 2D gas is created by trapping atoms very tightly in one dimension (the \(z\) axis) such that the motion in the \(z\) direction is effectively frozen out. The effective 2D scattering length for such a gas is given by \([11, 12]\)

\[
a_{2D} = \frac{4}{\pi} \frac{\hbar}{B} l_z \exp \left(-\sqrt{\frac{\pi}{2m\omega_z} a_{3D}}\right),
\]

where \(B \approx 0.915\), \(a_{3D}\) is the 3D \(s\)-wave scattering length, and \(l_z = \sqrt{\hbar/2m\omega_z}\) is the typical width of the system in the \(z\) direction. The 2D scattering length therefore depends not only on the 3D scattering length, but also upon the degree of confinement in the \(z\) direction.

Equation (3) shows that the coupling parameter for a 2D homogeneous Bose gas depends on the chemical potential of the system (and hence the density) as well as the 2D scattering length. This is in contrast with the case in 3D where the coupling parameter depends only upon the scattering length to first order.

3. The GPE in trapped 2D systems

The expression for the 2D coupling parameter shown in equation (2) was derived for a homogeneous system, and the correct application of these results to the case of a trapped gas is the main objective of this paper. In a previous paper \([7]\) we provided solutions of the 2D GPE in a trap using the homogeneous coupling parameter of equation (3) in order to illustrate the effect of the energy dependence of \(g_{2D}\). In this paper we focus on a more accurate description of the scattering in inhomogeneous systems.

We consider a 3D Bose gas confined tightly in one dimension and weakly in the remaining two dimensions on a length scale \(\ell_{\text{trap}}\). A collision between two condensate particles will typically occur over some length scale \(\ell_{\text{coll}}\). Provided that \(\ell_{\text{coll}}\) is much smaller than \(\ell_{\text{trap}}\) we can use a local density approximation.

\(\dagger\) Note that this definition of \(a_{2D}\) differs slightly from that in our earlier work such that our \(a_{2D}\) here equals \(a_{2D}e^{\gamma_{\text{EM}}}\) in the notation of reference \([10]\). The definition used here simplifies the form of equation (2).
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We can introduce the length scale $\ell_{\text{coll}}$ by the following simple argument. We model the pair wave function of two atoms in the medium by that of a single particle with the reduced mass moving in a potential which consists of a circularly symmetric box of radius $L$ and a hard sphere of radius $a$ located in the centre of the box. For $s$-wave scattering the wave function is solved by

$$\psi(r) = A_0 J_0(\kappa r) + B_0 N_0(\kappa r),$$

where $J_0$ and $N_0$ are Bessel functions of the first and second kind respectively. In the zero-energy, zero-momentum limit we get $\psi(r) = A_0 + B_0 \ln(r)$. Applying the boundary conditions that the wave function vanishes on the radius $r = a$ and reaches the asymptotic value $\chi$ at the edge of the box gives

$$\psi(r) = \frac{\ln(r/a)}{\ln(L/a)} \chi$$ \text{ for } \alpha < r < L. \tag{6}

The extra energy caused by the curvature of this wave function resulting from the presence of the scattering potential is

$$\Delta E = \frac{\hbar^2}{2m} \int_a^L |\nabla \psi(r)|^2 d^2r = \frac{\hbar^2 |\chi|^2}{2m} \frac{2\pi}{\ln(L/a)}. \tag{7}

This energy depends upon the size of the box $L$, which is indeed the length scale relevant for the scattering of two particles in 2D. The scattering of two particles in a many-body system should obviously not depend on the size of the system as a whole when $L$ becomes large, and so we must interpret $L$ as the physically relevant length scale $\ell_{\text{coll}}$. The appropriate length scale over which a many-body wave function changes is the healing length $\ell_h$, given in homogeneous Bose condensed systems by $\ell_h = \hbar/\sqrt{2m\Delta g_{2D}n_0} = \hbar/\sqrt{2m\mu}$, and so it is this which must be used in equation (7).

Since $N_0|\chi|^2$ corresponds to the condensate density $n_0$, this leads in the homogeneous limit to a pair interaction strength of the form of equation (8).

The same argument can be applied straightforwardly to trapped gases if the condensate density varies slowly on the scale of the healing length, which is true except in the surface region. In this case, many-body effects cause the pair wave function to reach its asymptotic value on a length scale equal to the local healing length $\ell_h = \hbar/\sqrt{2m\Delta g_{2D}(r)n_0(r)}$. The two-body interaction strength is therefore given from equation (8) by replacing $\mu$ with $n_0(r)g_{2D}(r)$ producing a density-dependent effective interaction. Such density dependent coupling parameters are expected from the results of density functional theory which predict that the energy of the system is a functional of the density only.

In an inhomogeneous system the density is spatially dependent and thus the coupling parameter is also spatially dependent. In terms of the condensate wave function the density is given by $n_0(r) = N_0|\psi(r)|^2$. Equation (8) now gives for the coupling parameter the result

$$g_{2D}(r) = -\frac{4\pi\hbar^2}{m} \frac{1}{\ln(N_0|\psi(r)|^2g_{2D}(r)ma_{2D}^2/4\hbar^2)}. \tag{9}

An approximate solution to this equation may be found by iteration, giving

$$g_{2D}(r) = -\frac{4\pi\hbar^2}{m} \left[\ln(N_0\pi|\psi(r)|^2a_{2D}^2)\right]^{-1} + O\left(\frac{\ln|\ln(n_0a_{2D}^2)|}{\ln(n_0a_{2D}^2)}\right). \tag{10}

The first order term in this expansion agrees with the form of coupling parameter proposed by Kolomeisky et al. who used the renormalization group to analyse...
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a 2D homogeneous Bose gas. Earlier work by Shevchenko [15] also proposed such a coupling parameter based on the work of Schick [16]. More recently Tanatar et al. [17] have also made use of this approximation. Unfortunately the expansion in equation (9) is not valid for realistic systems since the higher order terms are not in general negligible, as will be shown in the following section.

A more accurate procedure would be to solve equation (8) numerically for $g_{2D}(n_0(r))$ and use this exact solution in solving the GPE. In the following section we present results which suggest that this accurate solution may be necessary in some circumstances.

4. Solutions to the Gross-Pitaevskii Equation

In this section we present numerical solutions of the 2D GPE for a Bose condensate trapped in a circularly symmetric, harmonic potential characterized by an angular frequency $\omega$. The various approximation schemes for the coupling parameter discussed in the previous section will be compared to the more accurate $g_{2D}(r)$ found from the numerical solution of equation (8). In order to illustrate our results, we choose as our parameters $\omega = 2\pi \times 100\text{Hz}$ and $a_{2D} = 6\text{nm}$. This 2D scattering length is approximately the 3D scattering length found for $^{87}\text{Rb}$, and so from equation (4) this corresponds to a situation where $l_z \approx a_{3D}$, and hence the two-dimensional nature of the scattering is important [7]. For these parameters the results we obtain correspond to healing lengths between $0.1\ell_{\text{trap}}$ and $0.5\ell_{\text{trap}}$ (for the very low $\mu$ solutions) at the centre of the trap. These healing lengths are sufficiently small for the local density approximation to be valid.

We will solve the GPE for three different approximations for the coupling parameter. The simplest case restricts $g_{2D}(r)$ to be constant everywhere and determined by equation (3) as in our earlier work [7]. Spatial variations can most simply be introduced by using the first term of the expansion in equation (9), which corresponds to the results of Kolomeisky et al. [8, 14]. Finally, the most accurate approximation is obtained using the full numerical solution of equation (8). Figure 1 provides sample solutions of the ground state wave functions and coupling parameters calculated using these three different approximations for the same chemical potential. It can be seen that, although the wave functions are fairly similar, the coupling parameters behave quite differently. The results for the constant coupling parameter agree well with the predictions of equation (8), and differ significantly only towards the edge of the condensate. Of course, this is to be expected since $\mu \approx n_0g_{2D}(r)$ near the centre of the trap. The energy contribution due to interactions for atoms on the edge of the condensate is greater with the constant coupling parameter than with either of the spatially varying parameters, and hence the constant parameter wave function has a lower amplitude in these surface regions.

Figure 1 does show a large difference between the two spatially dependent coupling parameters, however, especially in the central region where the condensate density is greatest. The coupling parameter of equation (8) is greater by about a third at the centre of the condensate than the full expression of equation (8), and remains larger throughout. This arises because the expansion of equation (8) does not converge sufficiently rapidly. Indeed, for the case illustrated here, the second order term in the expansion (which is negative) reaches a magnitude of approximately $-1$ at the centre of the trap (in the units used in figure 1).

Such large differences in the coupling parameters can lead to problems when
Figure 1. (a) Wave functions $\psi(r)$, and (b) coupling parameters $g(r)$ calculated for $\mu = 25\hbar\omega$. The dash-dot lines correspond to equation (3), the dashed lines correspond to equation (9), while the solid lines represent the full numerical solution of equation (8).
Solutions of the Gross-Pitaevskii equation in two dimensions calculating related quantities, such as condensate populations. Figure 2 shows the results for condensate populations versus chemical potentials calculated with each of the coupling parameters. As can be seen the predictions obtained using the approximation of equation (9) underestimate the condensate numbers by roughly 20 per cent compared to the full numerical solution of equation (8). This is a consequence of the greater strength of the coupling parameter which occurs in this approximation. Agreement between equations (8) and (9) is poor even though the usual criterion for a dilute gas \( n_0 a_{2D}^2 \ll 1 \) is obeyed \( n_0 a_{2D}^2 \) is of the order of \( 10^{-4} \) for the situation illustrated in figure 1. Indeed, in order to apply the approximation in equation (9) we require that \( \ln(n_0 a_{2D}^2) \gg 1 \) (while \( n_0 a_{2D}^2 < 1 \)), which is a much more stringent criterion, and one that is experimentally unfeasible requiring at least \( n_0 a_{2D}^2 \lesssim 10^{-20} \). For this reason the use of the full expression in equation (8) is necessary to simulate real 2D gases.

The spatially-constant approximation to the coupling parameter gives comparatively much better agreement with the full numerical solution in figure 2, although it also underestimates the condensate number by about 5 per cent. It would appear from these results therefore that if a simple analytical approximation of \( g_{2D} \) is required to estimate bulk properties of the system then the spatially constant approximation is preferable to equation (9). Of course the spatially constant approximation does not deal with the boundary regions of the condensate well, and so for properties dominated by edge effects the better analytical approximation is likely to be that of equation (9).

The wave functions for vortex states can also be obtained in 2D, if we assume a solution of the form

\[
\psi(\mathbf{r}) = \phi(\mathbf{r}) e^{i\kappa \theta},
\]

(10)

where \( \theta \) is the angle around the vortex core, and \( \kappa \) is an integer. The phase of \( \psi \) therefore wraps around by \( 2\pi \kappa \) as the range of \( \theta \) is traversed. The energy per particle (in a non-rotating frame) for a condensate with wave function \( \psi \) is given by the functional

\[
E[\psi] = \int d\mathbf{r} \left[ \frac{\hbar^2}{2m} |\nabla \psi(\mathbf{r})|^2 + V_{\text{trap}}(\mathbf{r})|\psi(\mathbf{r})|^2 + \frac{N_0 g_{2D}(\mathbf{r})}{2} |\psi(\mathbf{r})|^4 \right].
\]

(11)

Creation of a vortex in the centre of the trap comes at the cost of increasing the contributions from both the kinetic energy and the trapping potential terms in the energy functional, although the interaction term is reduced by virtue of a lower central density. The single vortex state can be made energetically favourable by rotating the trap at a frequency \( \Omega \) such that \( E[\psi_{\kappa=0}] \) becomes less than \( E[\psi_{\kappa=1}] - \Omega N_0 \hbar \kappa \). The point at which this occurs is known as the thermodynamic critical frequency \( \Omega_c \), and this is shown in figure 3 for the various forms of \( g_{2D} \). The 2D critical frequency is substantially lower than for a 3D gas with the same scattering length \( (a_{3D} = a_{2D}) \) due principally to the much higher interaction strength which occurs in 2D. In figure 3b it can be seen that the effect of a density-dependent coupling parameter is to reduce the critical frequency as compared to the constant parameter case. This is to be expected since the appearance of a vortex lowers the mean density of the condensate, which decreases the coupling parameter calculated from either of equations (5) or (4). The lower coupling parameter means a greater saving in the interaction energy term when a vortex is created and therefore decreases the critical frequency. The saving in the interaction energy is due principally to the reduction of the density in the centre of the condensate where the density (and hence coupling parameter) is greatest in the ground state. Because the ground
Figure 2. a) Condensate numbers as a function of chemical potential in 2D for various coupling parameters. b) The percentage differences in the condensate populations as compared to the full numerical solution. The line styles correspond to those used in figure [1].
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Figure 3. a) Critical frequency versus condensate number for 2D and 3D condensates. The upper curve corresponds to the 3D case with $a_{3D} = a_{2D}$, whilst the lower curves represent the various 2D results. b) A detailed view of the critical frequencies in 2D using the three forms of the coupling parameter discussed. The line styles correspond to those used in figure 1.

state coupling parameter is much larger in the approximation of equation (9), the interaction energy saving is also greater. The critical frequency is therefore lower in this approximation compared to the results obtained using the coupling parameter of equation (8). In contrast to the spatially dependent $g_{2D}$ cases, the spatially-constant coupling parameter calculated from equation (3) increases when a vortex is formed, due to the greater chemical potential of the vortex state, and so the critical frequency is higher in this approximation.
5. Conclusions

In this paper we have applied previous results obtained for the many-body T-matrix in a homogeneous condensate to the more currently relevant problem of a trapped condensate, by means of a local density approximation. This leads to a spatially dependent coupling parameter appearing in the non-linear term of the Gross-Pitaevskii equation. We have shown that results obtained using the full numerical solution to the coupling parameter can differ substantially from the simple first approximation obtained via a series expansion. The form of the coupling parameter in this approximation is the same as that presented in recent work by Kolomeisky et al. [8, 14], Tanatar et al. [17], and Shevchenko [15], and is closely related to the work of Schick [16]. However, this approximation is only valid in the limit \( \ln(n_0a^2_{2D}) \gg 1 \) (while \( n_0a^2_{2D} < 1 \)) which is not experimentally relevant. Our results indicate that the full expression of equation (8) may be needed to model current experiments accurately. Corrections to equation (8) are expected to be of order \( (n^3a^2_{2D}) \ln(na^2_{2D}) \), and the limit where this parameter is small should be experimentally relevant.

Agreement with the full numerical solution for the coupling parameter is found to be substantially better if it is approximated using a spatially constant (but energy dependent) parameter as in the homogeneous limit. It would seem from the results presented here that if an approximate analytical form of the coupling parameter is required (for deriving approximate Thomas-Fermi wave functions for example) then the spatially constant form of \( g_{2D} \) given in equation (8) is preferable to the expression of equation (9) for many purposes.

Acknowledgments

We would like to thank K. Burnett and M.J. Davis for useful discussions. This research was supported by the Engineering and Physical Sciences Research Council of the United Kingdom, and by the European Union via the “Cold Quantum Gases” network. In addition, M.D.L. was supported by the Long Studentship from The Queen’s College, Oxford, and S.A.M. would like to thank the Royal Society for financial support.

References

[1] Görlitz A, Vogels J M, Leinhard A E, Raman C, Gustavson T L, Abo-Shaeer J R, Chikkatur A P, Gupta S, Inouye S, Rosenband T and Ketterle W 2001 Phys. Rev. Lett. 87 130402
[2] Zobay O and Garraway B M 2001 Phys. Rev. Lett. 86 1195
[3] Gauck H, Hartl M, Schneble D, Schützler H, Pfau T and Mlynek J 1998 Phys. Rev. Lett. 81 5298
[4] Hinds E A, Boshier M G and Hughes I G 1998 Phys. Rev. Lett. 80 645
[5] Hohenberg P C 1967 Phys. Rev. 158 383
[6] Bagnato V and Kiepner D 1991 Phys. Rev. A 44 7439
[7] Lee M D, Morgan S A, Davis M J and Burnett K 2002 Phys. Rev. A 65 043617
[8] Kolomeisky E B, Newman T J, Straley J P and Qi X 2000 Phys. Rev. Lett. 85 1146
[9] Taylor J R 1972 Scattering Theory (New York: Wiley)
[10] Morgan S A, Lee M D and Burnett K 2002 Phys. Rev. A 65 022706
[11] Petkov D S, Holzmann M and Shlyapnikov G V 2000 Phys. Rev. Lett. 84 2551
[12] Petkov D S and Shlyapnikov G V 2001 Phys. Rev. A 64 012706
[13] Nunes G S 1999 J. Phys. B: At. Mol. Opt. Phys. 32 4293
[14] Kolomeisky E B and Straley J P 1992 Phys. Rev. B 46 11749
[15] Shevchenko S I 1992 Sov. J. Low Temp. Phys. 18 223
[16] Schick M 1971 Phys. Rev. A 3 1067
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[17] Tanatar B, Minguzzi A, Vignolo P and Tosi M 2002 Preprint cond-mat/0205064