Chapter 3
Gross-Pitaevskii Model of the Condensate

Abstract The Gross-Pitaevskii equation (GPE) is a successful and well-established model for describing an atomic Bose-Einstein condensate. Here we introduce this model, along with its assumptions. Throughout the rest of this chapter we explore its properties and key time-independent solutions.

3.1 The Gross-Pitaevskii Equation

We assume that the gas is at zero temperature, such that the thermal gas and thermally-driven excitations of the condensate are non-existent. This is valid for $T \ll T_c$, which is often satisfied in BEC experiments. In any real gas, the particles also interact with each other, deviating from the ideal gas predictions of Chap. 2. Particle interactions amplify the fluctuations in any quantum field (so-called "quantum fluctuations"); these excite particles out of the ground state and deplete the condensate. An exact description of N interacting quantum particles would proceed by parameterising the system by an N-body wavefunction, $\mathbf{\Psi}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t)$, which obeys the many-body Schrödinger equation. However, the complexity of this approach makes it intractable for modelling more than a few particles, let alone the thousands or millions typical of an atomic BEC.

Fortunately, the interactions in atomic BECs are weak; this is due to their extreme diluteness and the weak forces between neutral atoms. As such, quantum fluctuations have a weak effect on the condensate, and will be ignored. Then, and assuming a large number of particles ($N \gg 1$), the many-body wavefunction can be approximated by an effective single-particle wavefunction, $\Psi(\mathbf{r}, t)$. Given the physical picture of the condensate as a giant matter wave (see Sect. 2.5.6), it is natural to describe it via a single wavefunction. This *macroscopic wavefunction* is a complex field that can be written as,

$$\Psi(\mathbf{r}, t) = \sqrt{n(\mathbf{r}, t)} \exp\left[iS(\mathbf{r}, t)\right], \tag{3.1}$$

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where n and S are the density and phase distributions of the condensate, and is normalized to N atoms, i.e.,

$$\int |\Psi|^2 \, \mathrm{d}^3\mathbf{r} = N. \tag{3.2}$$

In the absence of interactions, this wavefunction would be governed by the single-particle Schrödinger equation, $i\hbar\partial\Psi/\partial t = [-(\hbar^2/2m)\nabla^2 + V(\mathbf{r}, t)]\Psi$, where ∇^2 is the Laplacian operator and $V(\mathbf{r}, t)$ is the potential acting on the wavefunction (which, in general, may depend on position and time). However, the governing equation must be modified to account for the interactions between atoms. The gas is sufficiently dilute that three-body (and higher) interactions are typically negligible. The dominant interactions are elastic two-body interactions arising from van der Waals forces between the neutral atoms. For two atoms at positions $\mathbf{r_1}$ and $\mathbf{r_2}$ this interaction is well-described by the contact (hard-sphere) interaction,

$$\mathcal{U}(\mathbf{r_1} - \mathbf{r_2}) = g\delta(\mathbf{r_1} - \mathbf{r_2}), \tag{3.3}$$

where δ is Dirac's delta function, and the coefficient g is given by,

$$g = \frac{4\pi\hbar^2 a_{\mathrm{s}}}{m}. \tag{3.4}$$

Here a_{s} is the *s-wave scattering length*, a quantity used in atomic physics for characterising the interactions of atoms in the low energy limit (for a detailed description see, e.g. Ref. [1]). For the two most common BEC atomic species, ^{87}Rb and ^{23}Na, $a_{\mathrm{s}} = 5.8$ and $2.8\,\mathrm{nm}$, respectively. While the true interaction potential between two atoms is more complicated, its detailed shape is unimportant provided that $a_{\mathrm{s}} \ll d$, where d is the average interparticle distance (or, equivalently, $na_{\mathrm{s}}^3 \ll 1$). Furthermore, within this picture, the condition for weak interactions is $a_{\mathrm{s}} \ll \lambda_{\mathrm{dB}}$.

Taking into account these interactions, the mean-field wavefunction $\psi(\mathbf{r}, t)$ can be shown to satisfy a modified Schrödinger equation called the *Gross-Pitaevskii equation*,

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(\mathbf{r}, t)\Psi + g|\Psi|^2\Psi. \tag{3.5}$$

The formal derivation of the GPE is beyond our scope but can be found in, e.g. [1–3]. The first two terms on the right-hand side are familiar from the Schrödinger equation, accounting for kinetic and potential energy. The cubic term $g|\Psi|^2\Psi$ arises from the atomic interactions and makes the equation *nonlinear*. Similar *Nonlinear Schrödinger Equations (NLSEs)* arise in optics, plasma physics and water waves. In one spatial dimension, the NLSE has special mathematical properties, such as soliton solutions and infinite conservation laws (see Chap. 4). The physical interpretation of the nonlinear term is that, at a given point in space, there is an energy contribution arising from the mean-field interactions of all the atoms in the immediate vicinity. The quantity g depends on the given atomic species and can be positive or negative.

Experimentalists can also control sign and magnitude of g using Feshbach resonances. Here magnetic fields are used to couple the two-body scattering to a bound state; when this coupling is close to some resonant magnetic field, huge changes in the two-body scattering properties are possible. For $g > 0$ the interactions are *repulsive*, for $g < 0$ the interactions are attractive, and for $g = 0$ there are no interactions (and the equation reduces to the Schrödinger equation). The case of repulsive interaction is the most studied, so, unless we explicitly specify the sign of g, we take $g > 0$ hereafter.

The GPE can also be extended to take thermal and quantum effects into account, and further information can be found in Refs. [4–6].

3.1.1 Mass, Energy and Momentum

The total mass of the condensate is $M = mN$, where N is provided by the normalization condition on Ψ, Eq. (3.2).

The energy is,

$$E = \int \left[\frac{\hbar^2}{2m} |\nabla \Psi|^2 + V|\Psi|^2 + \frac{g}{2}|\Psi|^4 \right] \mathrm{d}^3\mathbf{r} = E_{\text{kin}} + E_{\text{pot}} + E_{\text{int}}. \tag{3.6}$$

The terms represent (from left to right) *kinetic energy* E_{kin}, *potential energy* E_{pot} and *interaction energy* E_{int}. Providing that the potential V is independent of time, then the energy $E = E_{\text{kin}} + E_{\text{pot}} + E_{\text{int}}$ is conserved during the time evolution of the condensate.

It can be useful, particularly when determining the energy numerically, to define $\Psi = \Psi_{\text{r}} + i\Psi_{\text{i}}$, where Ψ_{r} and Ψ_{i} are the real and imaginary parts of the wavefunction. Then, the $|\nabla\Psi|^2$ term in the energy can be expressed in a more convenient form, $|\nabla\Psi|^2 = (\nabla\Psi_{\text{r}})^2 + (\nabla\Psi_{\text{i}})^2$.

Meanwhile the momentum of the condensate is,

$$\mathcal{P} = \frac{i\hbar}{2} \int \left(\Psi \nabla \Psi^* - \Psi^* \nabla \Psi \right) \mathrm{d}^3\mathbf{r}. \tag{3.7}$$

3.2 Time-Independent GPE

Time-independent solutions of the GPE satisfy,

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) e^{-i\mu t/\hbar}, \tag{3.8}$$

where μ is a constant called the *chemical potential*. The exponential term represents the freedom for the phase to freely evolve with time, uniformly across the system, while the density $n(\mathbf{r}, t) = |\psi(\mathbf{r})|^2$ is unaffected. Inserting Eq. (3.8) into Eq. (3.5), we obtain the *time-independent GPE* for the time-independent wavefunction $\psi(\mathbf{r})$,

$$\mu\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{r})\psi + g|\psi|^2\psi. \tag{3.9}$$

Note that the potential V must be independent of time here. Solutions of the time-independent GPE are stationary solutions of the system, and the lowest energy solution is the ground state of the BEC. $\psi(\mathbf{r})$ is real for the simple solutions that we discuss in this Chapter.

The chemical potential is the eigenvalue of time-independent GPE, and direct integration leads to the expression,

$$\mu = \frac{1}{N}(E_{\text{kin}} + E_{\text{pot}} + 2E_{\text{int}}). \tag{3.10}$$

In the absence of interactions, this reduces to the energy per particle, consistent with the eigenvalue of the time-independent Schrödinger equation. More generally, the chemical potential is defined as $\mu = \partial E/\partial N$.

3.3 Fluid Dynamics Interpretation

There is a deep link between the GPE and fluid dynamics. Indeed, we can picture the condensate as a fluid, characterised by its density and velocity distributions. From the earlier relation, $\Psi(\mathbf{r}, t) = \sqrt{n(\mathbf{r}, t)}e^{iS(\mathbf{r},t)}$ (known in this context as the *Madelung transform*) the number density follows as $n(\mathbf{r}, t) = |\Psi(\mathbf{r}, t)|^2$. From this relation we have also the *mass density* $\rho(\mathbf{r}, t)$ conventionally used in fluid dynamics, $\rho(\mathbf{r}, t) = m\, n(\mathbf{r}, t)$.

The fluid velocity field $\mathbf{v}(\mathbf{r}, t)$ is defined from the phase via,

$$\mathbf{v}(\mathbf{r}, t) = \frac{\hbar}{m}\nabla S(\mathbf{r}, t). \tag{3.11}$$

Using the Madelung transform $\Psi = \sqrt{n}e^{iS}$ and the above velocity relation, we find that the energy integral of Eq. (3.6) can be written as,

$$E = \int \left[\frac{\hbar^2}{2m}\left(\nabla\sqrt{n}\right)^2 + \frac{mnv^2}{2} + Vn + \frac{gn^2}{2}\right] \mathrm{d}^3\mathbf{r}. \tag{3.12}$$

The first two terms comprise the kinetic energy. The first of these is the quantum kinetic energy. It arises due to the zero-point motion of confined particles, and vanishes for a uniform system. The second term is the conventional kinetic energy associated with the flow of the fluid.

Inserting the Madelung transform into the GPE, and separating real and imaginary terms, we obtain two equations. The first is the classical *continuity equation*,

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0. \tag{3.13}$$

The continuity equation expresses conservation of the number of atoms (or, when written in terms of $\rho(\mathbf{r}, t)$, conservation of mass). By integrating the equation over a given volume, we see that, if the number of atoms changes in that volume, it is because fluid has moved in or out of it.

The second equation is,

$$m\frac{\partial \mathbf{v}}{\partial t} = -\nabla\left(\frac{1}{2}mv^2 + V + gn - \frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{n}}{\sqrt{n}}\right). \tag{3.14}$$

The $\nabla^2\sqrt{n}/\sqrt{n}$ term is termed the *quantum pressure* term (see below). With some manipulation, we can write this in the equivalent form,

$$mn\left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v}\right) = -\nabla(P + P') - n\nabla V, \tag{3.15}$$

where P and P' are respectively the *pressure* and the *quantum pressure*,

$$P = \frac{gn^2}{2}, \qquad P' = -\frac{\hbar^2}{4m}n\nabla^2(\ln n). \tag{3.16}$$

Equations (3.13) and (3.14) (or, equivalently, Eqs. (3.13) and (3.15)) are known as the *superfluid hydrodynamic equations*. They can also be written in index notation.[1]

Notice that the pressure depends only on the density. This property makes the condensate a *barotropic fluid*; as a consequence, surfaces of constant pressure are also surfaces of constant density. The quantum pressure is a pure quantum effect, and vanishes if we set Planck's constant equal to zero. It has the same origin as the quantum kinetic energy, i.e. zero point motion, which creates a pressure that opposes any 'squashing' or 'bending' of the condensate. In a uniform condensate the quantum pressure is zero because n is constant.

Equation (3.15) is very similar to the classical Euler equation for an inviscid fluid. To understand the relation between condensates and classical fluids, we compare the relative importance of pressure and quantum pressure. Using Eq. (3.16), we estimate

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[1] In index notation, Eqs. (3.13) and (3.15) are $\frac{\partial n}{\partial t} + \frac{\partial (nv_j)}{\partial x_j} = 0$ and $mn\left(\frac{\partial v_k}{\partial t} + v_j\frac{\partial v_k}{\partial x_j}\right) = -\frac{\partial P}{\partial x_k} - \frac{\partial P'_{jk}}{\partial x_j} - n\frac{\partial V}{\partial x_k}$, where v_j is the jth Cartesian component ($j = 1, 2, 3$) of the velocity $\mathbf{v}$, we have assumed summation over repeated indices, and that the components P'_{jk} of the quantum stress tensor P' are $P'_{jk} = -\frac{\hbar^2}{4m}n\frac{\partial^2(\ln n)}{\partial x_j \partial x_k}$.

that the order of magnitude of P and P' are respectively $P \sim gn^2$ and $P' \sim \hbar^2 n/m\xi^2$, where ξ is the length scale of the variations of n. Then $P'/P \sim \hbar^2/(mng\xi^2)$, and hence the quantum pressure becomes negligible ($P' \ll P$) in the limit of length scales larger than ξ. If in addition, the trapping potential is absent ($V = 0$) then Eq. (3.15) become negligible, and the equation reduces to the classical Euler equation, which describes the motion of a classical fluid without viscosity.

The lengthscale in question is provided by the *healing length*, defined as,

$$\xi = \frac{\hbar}{\sqrt{gmn}}. \tag{3.17}$$

The typical value of the healing length in atomic BECs is $\xi \sim 10^{-6}$ m; for superfluid helium (^{4}He) the healing length is much smaller, $\xi \sim 10^{-10}$ m.

3.4 Stationary Solutions in Infinite or Semi–infinite Homogeneous Systems

In experiments, atomic condensates are confined by bowl-like trapping potentials $V(\mathbf{r})$. Condensates are therefore small (typically of the order of 10^{-5} or 10^{-4} m) and inhomogeneous (the density depends on the position). However, many general properties of atomic condensates can be understood from the simpler scenario of a homogeneous condensate in an infinitely-sized or semi-infinitely-sized system. The homogeneous condensate is also a useful model of superfluid helium, as the sizes of the samples of ^{4}He typically used in experiments range from 10^{-2} to 10^{-1} m, many orders of magnitude larger than the healing length. A homogeneous condensate would not be stable for $g < 0$ (as we see later) and so we consider $g > 0$ for now.

3.4.1 Uniform Condensate

For $V = 0$ (uniform condensate of infinite extent), the stationary solution is uniform, and the time-independent GPE becomes,

$$\mu\psi = g|\psi|^2\psi. \tag{3.18}$$

The solution is then,

$$\psi = \psi_0 = \sqrt{\mu/g}. \tag{3.19}$$

The corresponding number and mass densities are, respectively,

$$n = n_0 = |\psi_0|^2 = \mu/g, \qquad \rho = \rho_0 = m\mu/g. \tag{3.20}$$

3.4.2 Condensate Near a Wall

Consider a *one-dimensional hard wall* defined by,

$$V(x) = \begin{cases} \infty & \text{for } x < 0, \\ 0 & \text{for } x \geq 0. \end{cases}$$

No atoms exist in the region $x < 0$ (since this would require infinite energy), and so the boundary condition at $x = 0$ is $\psi(0) = 0$. Away from the wall (in the positive x direction) the condensate must recover its bulk form, giving the second boundary condition that $\psi(x) \rightarrow \psi_0 = \sqrt{\mu/g}$ for $x \rightarrow \infty$. In the semi-infinite region $x \geq 0$ the one-dimensional (1D) time-independent GPE is,

$$\mu\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + g|\psi|^2\psi. \tag{3.21}$$

The solution of this equation which satisfies the boundary conditions is,

$$\psi(x) = \psi_0 \tanh\left(\frac{x}{\xi}\right). \tag{3.22}$$

The meaning of the healing length ξ is now apparent: it is the characteristic minimal distance over which ψ changes spatially. The 'healing' profile is supported at a wall by the balance between the kinetic energy term in the GPE and the interaction term. Denoting the spatial scale of the variation in the wavefunction as ξ, these terms are of the order of $\hbar^2/m\xi^2$ and gn_0, respectively. Equating these terms and rearranging leads to $\xi = \hbar/\sqrt{mn_0 g}$, the healing length as defined in Eq. (3.17). Note that the healing length is sometimes defined with a $\sqrt{2}$ in the denominator.

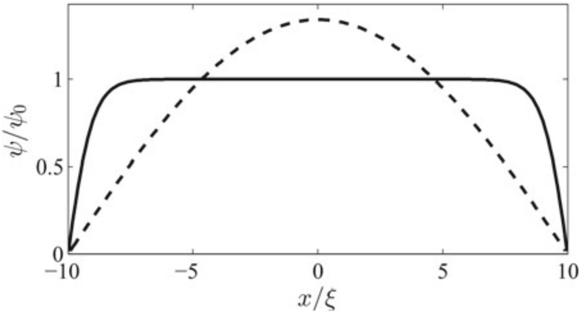

Fig. 3.1 Condensate wavefunction ψ (in units of ψ_0) as a function of position x (in units of ξ) within a 1D infinite square well of width (here with width 20ξ). Shown are the profiles for a non-interacting condensate ($g = 0$) and aAtomic condensates repulsively-interacting ($g > 0$) condensate. Note how the wavefunction "heals" at each boundary according to Eq. (3.22), recovering its bulk density at a distance from the wall of the order of few times the healing length ξ

In an infinite square well of width L_0, which is much wider than the healing length ($L_0 \gg \xi$), we then expect the wavefunction to 'heal' at each boundary, according to Eq. (3.22), and reach the bulk value in the centre of the well. This is shown in Fig. 3.1.

It is interesting to compare this to the case of $g = 0$, for which the ground state is given by the well-known solution of the Schrödinger equation for a particle in an infinite well, $\psi \sim \sin(\pi x/L_0)$. Clearly the interactions between the atoms broaden and flatten the density profile by increasing the energetic cost of concentrating atoms in one place.

3.5 Stationary Solutions in Harmonic Potentials

Atomic condensates are typically confined by harmonic potentials which may, in general, be anisotropic in space. For simplicity here we start by considering a spherically-symmetric harmonic trap,

$$V(\mathbf{r}) = \frac{m}{2}\omega_r^2 r^2, \tag{3.23}$$

where $r^2 = x^2 + y^2 + z^2$. The characteristic length scale of this potential is the *harmonic oscillator length*,

$$\ell_r = \sqrt{\hbar/m\omega_r}. \tag{3.24}$$

There is no general analytic solution for the ground state (lowest energy) solution of the BEC in a harmonic trap; usually the ground state is found by numerically solving Eq. (3.9). However, there exist useful analytic results for certain regimes which we describe below. It is useful to work in terms of the *interaction parameter*,[2] Na_s/ℓ_r. Below we distinguish the following cases: no interactions, strong repulsive interactions ($Na_\mathrm{s}/\ell_r \gg 1$) and weak interactions ($|Na_\mathrm{s}/\ell_r| \ll 1$).

3.5.1 No Interactions

In the absence of atomic interactions ($g = 0$) the time-independent GPE reduces to the Schrödinger equation,

$$\mu\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + \frac{m\omega_r^2 r^2}{2}\psi. \tag{3.25}$$

The ground state harmonic oscillator solution is well-known to be a three-dimensional Gaussian wave function,

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[2] More generally, for an anisotropic harmonic trap, the corresponding interaction parameter is $Na_\mathrm{s}/\bar{\ell}$, where $\bar{\ell} = \sqrt{\hbar/m\bar{\omega}}$ and $\bar{\omega} = (\omega_x\omega_y\omega_z)^{1/3}$ is the geometric mean of the trap frequencies.

$$\psi(\mathbf{r}) = \frac{N^{1/2}}{\pi^{3/4}\ell_r^{3/2}} \exp\left(-\frac{r^2}{2\ell^2}\right). \tag{3.26}$$

Using Eq. (3.6), one can show that this has the expected 3D harmonic oscillator energy $E = \frac{3}{2}N\hbar\omega_r$.

3.5.2 Strong Repulsive Interactions

Let the interactions be strongly repulsive, satisfying $Na_\mathrm{s}/\ell_r \gg 1$. We expect a condensate profile which is significantly broadened and flattened due to the repulsive interactions. An analytic solution is found if we neglect the $\nabla^2\psi$-term in the GPE; this is known as the *Thomas-Fermi approximation*. The time-independent GPE simplifies to,

$$\mu\psi = g|\psi|^2\psi + V\psi. \tag{3.27}$$

Substituting $n = |\psi|^2$ and $V(r) = \frac{1}{2}m\omega^2 r^2$, we obtain $n(r) = (2\mu - m\omega_r^2 r^2)/2g$. Density cannot be negative, so we assume that $n(r) = 0$ if $2\mu \leq m\omega_r^2 r^2$. The last equality defines the *Thomas-Fermi radius* R_r, which satisfies,

$$\mu = \frac{1}{2}m\omega_r^2 R_r^2. \tag{3.28}$$

We conclude that the Thomas-Fermi density profile is,

$$n(r) = \begin{cases} \dfrac{\mu}{g}\left(1 - \dfrac{r^2}{R_r^2}\right) = \dfrac{m\omega_r^2(R_r^2 - r^2)}{2g} & \text{if } r \leq R_r, \\ 0 & \text{if } r > R_r, \end{cases} \tag{3.29}$$

and has the shape of an inverted parabola. Provided that $Na_\mathrm{s}/\ell_r \gg 1$, the Thomas-Fermi solution is an excellent approximation of the solution of the GPE determined numerically, and compares well with experimental data, as shown in Fig. 3.2. Note, however, the slight deviation from the true numerical solution close to the condensate's edge; here the gradient terms, neglected within the Thomas-Fermi model, become significant.

The application of the normalization condition, Eq. (3.2), to the above solution and manipulation of the resulting expression leads to useful relations for the chemical potential and the energy of the condensate in terms of the number of atoms N,

$$\mu = \frac{\hbar\omega_r}{2}\left(\frac{15Na_\mathrm{s}}{\ell_r}\right)^{2/5}, \quad E = \frac{5}{7}\mu N. \tag{3.30}$$

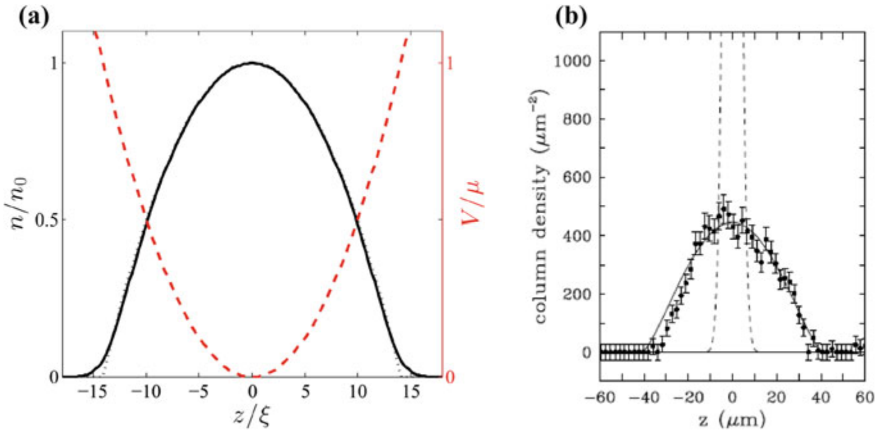

Fig. 3.2 **a** Density profile $n(z)$ plotted versus position z (in units of the healing length ξ). The agreement between the analytic Thomas-Fermi density profile (*dotted black line*) and the numerically-determined solution of the GPE (*solid black line*) is so good that the lines overlap everywhere but in the tails near $z \approx \pm 15\xi$. The harmonic trapping potential $V(z)$ is indicated by the dashed *red line*. **b** An experimental density profile, compared to the Thomas-Fermi prediction (*solid line*) and the non-interacting prediction (*dashed line*). Reprinted figure with permission from [7]. Copyright 1999 by the American Physical Society

The latter is obtained from the relation $\mu = \partial E/\partial N$. Since $Na_s/\ell_r \gg 1$, it is evident that in the Thomas-Fermi regime the chemical potential and energy per particle are considerably greater than the typical trap energy $\hbar\omega_r$.

In the more general case where the harmonic potential is anisotropic in space, $V(x, y, z) = m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)/2$, the Thomas-Fermi boundary is an ellipsoidal surface satisfying the equation,

$$\frac{x^2}{R_x^2} + \frac{y^2}{R_y^2} + \frac{z^2}{R_z^2} = 1, \tag{3.31}$$

where the three Thomas-Fermi radii R_x, R_y and R_z satisfy,

$$\mu = \frac{1}{2}m\omega_x^2 R_x^2 = \frac{1}{2}m\omega_y^2 R_y^2 = \frac{1}{2}m\omega_z^2 R_z^2. \tag{3.32}$$

In this anisotropic case, it is most convenient to write the density profile as,

$$n(x, y, z) = \begin{cases} \dfrac{\mu}{g}\left(1 - \dfrac{x^2}{R_x^2} - \dfrac{y^2}{R_y^2} - \dfrac{z^2}{R_z^2}\right), & \text{within the ellipsoid,} \\ 0 & \text{elsewhere.} \end{cases} \tag{3.33}$$

From this the anisotropic versions of the chemical potential and energy, Eq. (3.30), can be determined.

3.5.3 Weak Interactions

The following variational approach determines an approximate solution of the time-independent GPE in a harmonic potential when the interactions (either positive or negative) are weak, that is $|Na_\mathrm{s}/\ell_r| < 1$.

In the limiting case $g = 0$ we know that the exact wavefunction is the Gaussian harmonic oscillator ground state, Eq. (3.26). For weak interactions we assume the following trial wavefunction, or *ansatz*, which is Gaussian in shape but has variable width $\sigma\ell_r$,

$$\psi(\mathbf{r}) = \left(\frac{N}{\pi^{3/2}\sigma^3\ell_r^3}\right)^{1/2} \exp\left(-\frac{r^2}{2\sigma^2\ell_r^2}\right). \tag{3.34}$$

where σ is our *variational parameter*. If $g = 0$ then $\sigma = 1$, i.e. we recover the exact non-interacting result.

Using the energy integral (3.6), the energy of the ansatz is,

$$E(\sigma) = \hbar\omega_r N\left[\frac{3}{4\sigma^2} + \frac{3\sigma^2}{4} + \frac{1}{\sqrt{2\pi}}\left(\frac{Na_s}{\ell_r}\right)\frac{1}{\sigma^3}\right]. \tag{3.35}$$

From left to right, the terms in the bracket represent kinetic energy, potential energy and interaction energy. For a given system (i.e. for specific values of N, ω, a_s and ℓ_r), Eq. (3.35) tells us how the energy varies with σ. The variational solution is defined as the variational state with the lowest energy, i.e. the minimum of $E(\sigma)$; the corresponding width is denoted σ_min. Figure 3.3 plots $E(\sigma)$ for various values of the interaction parameter Na_s/ℓ. The behaviour is different depending on whether the interactions are repulsive or attractive:

- For **repulsive interactions** ($g > 0$), $E(\sigma)$ diverges to infinity for both $\sigma \to 0$ (due to the positive kinetic and interaction energies) and $\sigma \to \infty$ (due to the potential energy), with a global minimum in-between, corresponding to the variational ground state. If $g = 0$, $\sigma_\mathrm{min} = 1$, corresponding to the non-interacting Gaussian solution. For increasing g, σ_min increases, i.e., the condensate becomes wider.
- For **attractive interactions** ($g < 0$), $E(\sigma)$ now diverges to minus infinity as $\sigma \to 0$. This is due to the dominance of the negative interaction energy in this limit. The lowest energy solution is thus a wavepacket of zero width, i.e. an unstable collapsed state![3] However, for small $|Na_\mathrm{s}/\ell_r|$, a *local minimum* exists in $E(\sigma)$ at non-zero width, representing a stable condensate of finite size. For larger $|Na_\mathrm{s}/\ell_r|$,

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[3] In reality, the BEC does not quite collapse to zero width; at high densities, repulsive inter-atomic forces kick-in which cause the condensate to then explode outwards, an effect termed the *bosenova*.

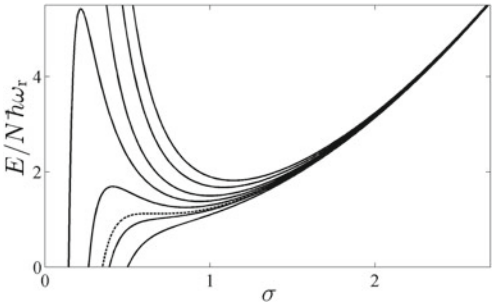

Fig. 3.3 Energy E (in units of $N\hbar\omega_r$) versus σ according to Eq. (3.35) for various values of the interaction parameter Na_s/ℓ_r corresponding, from *top* to *bottom*, to $[-1, -0.75, -0.67, -0.5, -0.25, 0, 0.5, 1]$. $Na_s/\ell_r = -0.67$ (*dashed line*) marks the critical point for the onset of collapse

the local minimum shifts to smaller widths; the attractive interactions cause the condensate to become narrower and more peaked. However, beyond some critical attractive interactions, the local minimum disappears and no stable solutions exist. In other words, all states collapse to zero width. The variational method predicts collapse to occur for $Na_s/\ell_r \leq -0.67$; this is close to the experimentally measured value of $Na_s/\ell_r \leq -0.64$. This tendency to collapse is the reason why repulsive condensates are more common and why we have avoided discussing condensates with attractive interactions so far.

Note that the above-assumed Gaussian profile is just an approximation. In the presence of repulsive interactions, the true condensate profile (e.g. as obtained by numerical solution of the GPE) is broader than a Gaussian (becoming more Thomas-Fermi like for increasing repulsive interactions), while for attractive interactions the shape is narrower and more peaked.

3.5.4 Anisotropic Harmonic Potentials and Condensates of Reduced Dimensionality

The shape of the condensate is determined by the shape of the trapping potential. A spherical harmonic potential induces a spherical condensate. It is also common to encounter elongated, or *cigar-shaped*, condensates and flattened, or *pancake-shaped*, condensates. The former case is achieved if the condensate is more tightly trapped in two directions, e.g. $\omega_x, \omega_y > \omega_z$, and the latter case, if it is more tightly trapped in one direction, e.g. $\omega_z > \omega_x, \omega_y$. These shapes are illustrated in Fig. 3.4.

By making these trap anisotropies more extreme, it is possible to engineer condensates of reduced dimensionality. Consider first a highly elongated trap ($\omega_x, \omega_y \gg \omega_z$). If the transverse trapping potential (which is of energy $\hbar(\omega_x\omega_y)^{1/2}$) is much larger

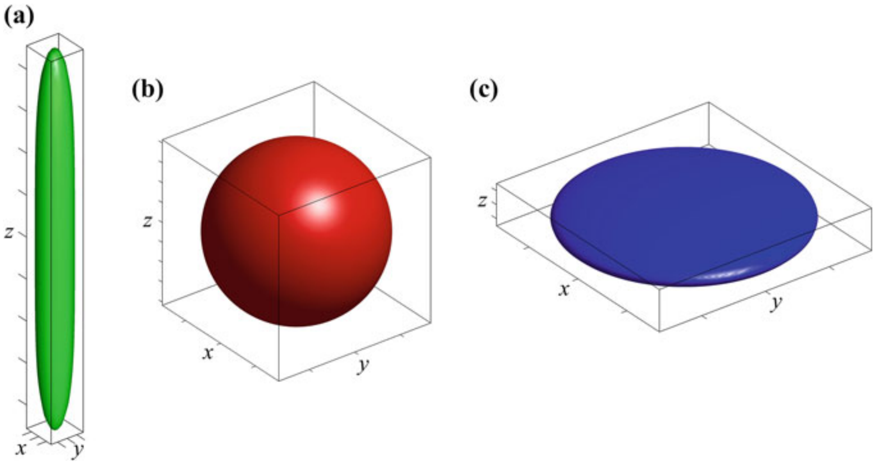

Fig. 3.4 The three most common condensate shapes that can be formed in an axisymmetric harmonic potential: **a** a cigar condensate ($\omega_x, \omega_y > \omega_z$), **b** a spherical condensate ($\omega_x = \omega_y = \omega_z$), and **c** a pancake condensate ($\omega_x, \omega_y < \omega_z$)

than the condensate energy scale (the chemical potential, μ), then excitations of the condensate in the x and y directions are highly suppressed, and the only significant dynamics occur in the z direction. The system has become effectively one-dimensional. An effectively two-dimensional condensate can be realized for $\omega_x, \omega_y \ll \omega_z$ and $\hbar\omega_z \gg \mu$.

In these limits the condensate can be described by suitable one-dimensional and two-dimensional GPEs. The reduction of the full three-dimensional GPE to these forms is straightforward, as we now outline for a one-dimensional system. Assuming the above criteria for an effectively one-dimensional condensate, we take the following ansatz for the condensate wavefunction,

$$\psi(x, y, z, t) = \psi_z(z, t)G_x(x)G_y(y). \tag{3.36}$$

In other words, we have decomposed ψ into independent components along x, y and z. Under the criterion $\hbar(\omega_x\omega_y)^{1/2} \gg \mu$ then the x and y component will be "locked" into the respective ground harmonic oscillator states, which are represented by the Gaussian functions,

$$G_x(x) = \frac{1}{(\pi\ell_x^2)^{1/4}}e^{-x^2/2\ell_x^2}, \qquad G_y(y) = \frac{1}{(\pi\ell_y^2)^{1/4}}e^{-y^2/2\ell_y^2}, \tag{3.37}$$

where $\ell_x = \sqrt{\hbar/m\omega_x}$ and $\ell_y = \sqrt{\hbar/m\omega_y}$ denote the harmonic oscillator lengths along x and y. The time-dependence now only appears in the axial wavefunction, ψ_z. Note that ψ_z is normalized to the number of atoms, i.e. $\int |\psi_z|^2 \, \mathrm{d}z = N$; as a result the transverse wavefunctions are both normalized to unity (leading to their pre-factors).

To obtain a 1D GPE, one proceeds by inserting the wavefunction ansatz (3.36) into the 3D GPE and manipulating. Since,

$$\frac{\mathrm{d}^2 G_x(x)}{\mathrm{d}x^2} = \left(\frac{x^2}{\ell_x^4} - \frac{1}{\ell_x^2}\right) G_x(x), \tag{3.38}$$

and similarly for $G_y(y)$, each term in the GPE acquires a $G_x(x)G_y(y)$ factor. To eliminate these factors, one multiplies the equation through by $G_x^* G_y^*$ (where * denotes complex conjugate) and integrates over all x and y. It is helpful to note that $\int_{-\infty}^{\infty} e^{-x^2} \mathrm{d}x = \sqrt{\pi}$. This leads to the following one-dimensional GPE for $\psi_z(z)$,

$$\mu_{1\mathrm{D}}\psi_z = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_z}{\mathrm{d}z^2} + g_{1\mathrm{D}}|\psi_z|^2\psi_z + \frac{1}{2}m\omega_z^2 z^2\psi_z. \tag{3.39}$$

Here $g_{1\mathrm{D}}$ and $\mu_{1\mathrm{D}}$ are the effective one-dimensional interaction strength and chemical potential, defined as,

$$g_{1\mathrm{D}} = \frac{g}{2\pi\ell_x\ell_y}, \qquad \mu_{1\mathrm{D}} = \mu - \frac{\hbar\omega_x}{2} - \frac{\hbar\omega_y}{2}. \tag{3.40}$$

Note that the trap geometries are often cylindrically symmetric, with $\omega_x = \omega_y$; this symmetry can simplify the integration steps.

Following similar arguments for an effectively two-dimensional condensate, one obtains the effective two-dimensional GPE for the two-dimensional wavefunction $\psi_{xy}(x, y, t)$,

$$\mu_{2\mathrm{D}}\psi_\perp = -\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2\psi_\perp}{\mathrm{d}x^2} + \frac{\mathrm{d}^2\psi_\perp}{\mathrm{d}y^2}\right) + g_{2\mathrm{D}}|\psi_\perp|^2\psi_\perp + \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2)\psi_\perp,$$

$$g_{2\mathrm{D}} = \frac{g}{\sqrt{2\pi}\ell_z}, \qquad \mu_{2\mathrm{D}} = \mu - \frac{\hbar\omega_z}{2}.$$

In this case the two-dimensional wavefunction is normalized according to $\int |\psi_\perp|^2 \, \mathrm{d}x\mathrm{d}y = N$.

In these one- and two-dimensional cases, the system energy is still described according to Eq. (3.6), with the gradient operator replaced by its one- and two-dimensional equivalents, and the integration taken over one and two dimensions, respectively. Moreover, the same analysis techniques presented for three-dimensional stationary solutions, e.g. the Thomas-Fermi approximation and the Gaussian variational approach, can be employed. In particular, the 1D GPE provides a simplified platform to study many generic properties of condensates, and, for example, its stationary solutions under hard-wall and periodic boundaries are well-established [8, 9]. Note, however, that the system stability can be significantly affected by the dimensionality of the system, for example, collapse under attractive interactions does not occur within the 1D GPE, as will be discussed further in Chap. 4.

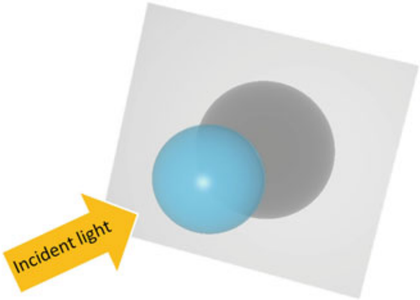

Fig. 3.5 Absorption imaging of a BEC. Laser light incident upon the BEC creates a shadow behind it, whose darkness is proportional to the column-integrated density of the BEC

3.6 Imaging and Column-Integrated Density

The most common approach to image a condensate is via optical absorption imaging. The condensate is illuminated by an uniform light beam from one side. The atoms absorb a proportion of the light such that a two-dimensional shadow is cast behind the condensate; this is recorded by camera as shown in Fig. 3.5, forming an *absorption image* of the condensate. Examples are the images in Fig. 1.4. Importantly, the darkness of the shadow is proportional to the atomic density, integrated along the direction light is travelling in[4]; we call this the *column-integrated density*.

To enable comparison between experimental absorption images and theoretical models, one must relate three-dimensional wavefunctions to the corresponding two-dimensional column-integrated density profiles. Assuming imaging in the z-direction, the column-integrated density n_{CI} is,

$$n_{\mathrm{CI}}(x, y) = \int_{-\infty}^{\infty} n(x, y, z)\, \mathrm{d}z. \tag{3.41}$$

3.7 Galilean Invariance and Moving Frames

A condensate in a homogeneous ($V = 0$) system satisfies the GPE,

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + g|\Psi|^2 \right) \Psi. \tag{3.42}$$

The stationary solution is $\Psi_0 = \sqrt{n_0} \exp\left[-i\mu t/\hbar\right]$, corresponding to a static ($\mathbf{v} = 0$) condensate. Now let us imagine, instead, that this condensate is moving with uniform velocity v_0 in the positive x direction, say. We can construct this moving solution as,

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[4] Fortunately, the atomic density is so low that scattering of the light beam is negligible and so the light effectively takes a direct path through the condensate.

$$\Psi = \Psi_0(x - v_0 t, y, z) \exp\left[i\frac{m v_0 x}{\hbar} - \frac{m v_0^2 t}{2\hbar} \right]. \tag{3.43}$$

Note that the density remains n_0 throughout. This is a demonstration of *Galilean invariance*, i.e. that the laws of physics are the same in all *inertial frames* (frames moving at fixed relative speed to each other). This is true only if the system is translationally invariant, i.e. the potential is the same everywhere.

Above, we imagine the condensate flowing at speed v_0 relative to the static observer (the *lab frame*). Instead, we can take the observer to be moving with the condensate. We can then write the *moving frame GPE*,

$$i\hbar\frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + g|\Psi|^2 + i\hbar v_0 \frac{\partial}{\partial \tilde{x}} \right)\Psi, \tag{3.44}$$

where $\tilde{x}$ is the x-coordinate in the moving frame and the Laplacian is evaluated in terms of the moving frame coordinates. In this moving frame, the flowing condensate solution of Eq. (3.43) is actually a stationary solution. It can be useful to work in the moving frame when modelling flows of condensates.

3.8 Dimensionless Variables

The typical numbers which appear in the GPE equation are very small and cumbersome, for example the reduced Planck's constant is $\hbar = 1.055 \times 10^{-34}$ Js. When numerically solving the GPE to model a condensate, it would be better if the numbers which we compute were of order unity; this minimises the role of floating point errors which are inherent to modern digital computation. Another problem is that not all the parameters which appear in the GPE are independent: identifying the truly independent parameters reduces the number of numerical simulations which are needed to understand the nature of the solution. It is therefore useful to introduce *dimensionless variables* and write the GPE in simpler *dimensionless form*. To illustrate the procedure, we consider two examples: homogeneous and harmonically-trapped condensates.

Before we start, we notice for the sake of generality that we are free to introduce the chemical potential μ in the time-dependent GPE by letting, in analogy with Eq. (3.8),

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}, t)e^{-i\mu t/\hbar}, \tag{3.45}$$

where now $\psi(\mathbf{r}, t)$ depends also on t; in other words, the exponential term takes care of part of (but not all of) the time dependence of the wavefunction. The resulting time-dependent GPE is,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + g|\psi|^2\psi + V\psi - \mu\psi. \tag{3.46}$$

3.8.1 Homogeneous Condensate

In the absence of trapping ($V = 0$), the governing equation is

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + g|\psi|^2\psi - \mu\psi. \tag{3.47}$$

We have seen that the wavefunction of a uniform condensate at rest is $\psi_0 = \sqrt{\mu/g}$, corresponding to the number density $n_0 = \mu/g$. We have also seen that the characteristic minimum distance over which the wavefunction varies is the healing length $\xi = \hbar/\sqrt{m\mu}$. Therefore the quantities n_0 and ξ are convenient units of density and length. Similarly, it is apparent from Eq. (3.8) or Eq. (3.45) that $\tau = \hbar/\mu$ is the natural unit of time. These remarks suggest the introduction of the following dimensionless variables (hereafter denoted by primes):

$$x' = \frac{x}{\xi}, \qquad y' = \frac{y}{\xi}, \qquad z' = \frac{z}{\xi}, \tag{3.48}$$

(in other words, $\mathbf{r}' = \mathbf{r}/\xi$), and

$$t' = \frac{t}{\tau}, \qquad \psi' = \frac{\psi}{\psi_0}. \tag{3.49}$$

To begin substituting these new variables into the GPE, we need to develop relations for their derivatives. Using the chain rule,

$$\frac{\mathrm{d}}{\mathrm{d}x} = \frac{1}{\xi}\frac{\mathrm{d}}{\mathrm{d}x'}, \quad \frac{\mathrm{d}}{\mathrm{d}y} = \frac{1}{\xi}\frac{\mathrm{d}}{\mathrm{d}y'}, \quad \frac{\mathrm{d}}{\mathrm{d}z} = \frac{1}{\xi}\frac{\mathrm{d}}{\mathrm{d}z'}, \quad \frac{\mathrm{d}}{\mathrm{d}t} = \frac{1}{\tau}\frac{\mathrm{d}}{\mathrm{d}t'}. \tag{3.50}$$

Hence the gradient and Laplacian operators acting on the primed variables are defined as,

$$\nabla = \frac{1}{\xi}\nabla', \quad \nabla^2 = \frac{1}{\xi^2}\nabla'^2. \tag{3.51}$$

Introducing these relations, Eq. (3.47) becomes the following *dimensionless GPE*,

$$i\frac{\partial\psi'}{\partial t'} = -\frac{1}{2}\nabla'^2\psi' + |\psi'|^2\psi' - \psi'. \tag{3.52}$$

This equation contains no parameters - it has been simplified to its mathematical essence.[5] These units are often termed *natural* or *healing length* units.

3.8.2 Harmonically-Trapped Condensate

Here we assume that the condensate is confined by a spherical harmonic trap $V = m\omega_r^2 r^2/2$. Then the governing equation is,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + g|\psi|^2\psi + V\psi - \mu\psi. \tag{3.53}$$

In this case the natural units of length and time are based on the harmonic oscillator length $\ell_r = \sqrt{\hbar/m\omega_r}$ and the inverse of the trap frequency, ω_r^{-1}. We set $\mathbf{r}' = \mathbf{r}/\ell$ (that is to say $x' = x/\ell$, $y' = y/\ell$ and $z' = /\ell$) and $t' = t/\tau$, where $\tau = 1/\omega_r$.

It is conventional with these units to define the dimensionless wavefunction ψ' as being normalized to unity, i.e.,

$$\int |\psi'|^2 \mathrm{d}^3\mathbf{r}' = 1. \tag{3.54}$$

Comparing to Eq. (3.2) and noting that $\mathrm{d}^3\mathbf{r} = \ell_r^3 \mathrm{d}^3\mathbf{r}'$, it follows that $\psi = (N/\ell_r^3)^{1/2}\psi'$.

Introducing these relations into Eq. (3.58) we arrive at the dimensionless form,

$$i\frac{\partial\psi'}{\partial t'} = -\frac{1}{2}\nabla'^2\psi' + C|\psi'|^2\psi' + \frac{r'^2}{2}\psi' - \mu'\psi'. \tag{3.55}$$

where $\mu' = \mu/\hbar\omega_r$ and,

$$C = \frac{4\pi a_s N}{\ell}. \tag{3.56}$$

is a dimensionless interaction parameter. These units are often termed *harmonic oscillator units*. For anisotropic harmonic traps, the harmonic units can be defined instead in terms of one of the trap frequencies or their geometric mean, $\bar{\omega} = (\omega_x\omega_y\omega_z)^{1/3}$.

Problems

3.1 (a) Using the normalization condition, determine the dimensions of the wavefunction Ψ in S.I. units (metres, kilograms, seconds).

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[5] In the literature, after transforming the GPE into dimensionless form, it is common to drop the primes.

(b) Verify that all terms of the GPE have the same dimension.
(c) Show that $g|\Psi|^2$ has dimension of energy.

3.2 Consider a BEC in the Thomas-Fermi limit, confined within a three-dimensional spherical harmonic trap.
(a) Normalize the wavefunction, and hence determine an expression for the Thomas-Fermi radius R_r in terms of N, a_s and ℓ_r.
(b) Determine an expression for the peak density in terms of N and R_r.
(c) Find an expression for the ratio R_r/ℓ_r, and comment on its behaviour for large N.
(d) What is the energy of the condensate?

3.3 Derive the expression for the variational energy of a three-dimensional trapped condensate, Eq. (3.35). Repeat in two dimensions (for a potential $V(x, y) = m\omega_r^2(x^2 + y^2)/2$) and in one dimension (for a potential $V(x) = m\omega_r^2 x^2/2$). For each case plot $E/N\hbar\omega_r$ versus the variational width σ, for some different values of the interaction parameter Na_s/ℓ_r. What effect does dimensionality have on the shape of the curves? How do this change the qualitative behaviour described in Sect. 3.5.3?

3.4 Consider a BEC in the non-interacting limit with wavefunction

$$\psi(x, y, z) = \sqrt{n_0}\, e^{-x^2/2\ell_x^2} e^{-y^2/2\ell_y^2} e^{-z^2/2\ell_z^2}, \tag{3.57}$$

where n_0 is the peak density and ℓ_x, ℓ_y and ℓ_z are the harmonic oscillator lengths in three Cartesian directions. The BEC is imaged along the z-direction. Determine the form of the column-integrated density $n_\mathrm{CI}(x, y)$. Hint: $\int_0^\infty e^{ax^2} = \frac{1}{2}\sqrt{\pi/a}$.

3.5 Consider a 1D uniform static condensate with $V(x) = 0$. Obtain an expression for the energy E in a length L of the condensate, in terms of n_0, g and L.

Now consider the condensate to be flowing with uniform speed v_0, by constructing a solution according to Eq. (3.43). Show that the solution satisfies the 1D GPE, and confirm that the velocity field of this solution is indeed $v(x) = v_0$. What is the corresponding energy for the flowing condensate, and how does it differ from the static result? Finally, what is its momentum?

3.6 Consider a homogeneous condensate. Identify dimensionless variables so that the dimensionless GPE is,

$$i\frac{\partial \psi'}{\partial t'} = -\nabla'^2\psi' + |\psi'|^2\psi' - \psi', \tag{3.58}$$

i.e., without the 1/2 factor as in Eq. (3.52).

References

1. C.J. Pethick, H. Smith, *Bose-Einstein Condensation in Dilute Gases* (Cambridge University Press, Cambridge, 2008)
2. J.F. Annett, *Superconductivity, Superfluids and Condensates* (Oxford University Press, Oxford, 2004)
3. L.P. Pitaevskii, S. Stringari, *Bose-Einstein Condensation (International Series of Monographs on Physics)* (Oxford Science Publications, Oxford, 2003)
4. N.P. Proukakis, B. Jackson, J. Phys. B **41**, 203002 (2008)
5. P.B. Blakie, A.S. Bradley, M.J. Davis, R.J. Ballagh, C.W. Gardiner, Adv. Phys. **57**, 363 (2008)
6. N.P. Proukakis, S.A. Gardiner, M. Davis, M. Szymańska (eds.), *Quantum Gases: Finite Temperature and Non-Equilibrium Dynamics* (Imperial College Press, London, 2013)
7. F. Dalfovo, S. Giorgini, L.P. Pitaevskii, S. Stringari, Rev. Mod. Phys. **71**, 463 (1999)
8. L.D. Carr, C.W. Clark, W.P. Reinhardt, Phys. Rev. A **62**, 063610 (2000)
9. L.D. Carr, C.W. Clark, W.P. Reinhardt, Phys. Rev. A **62**, 063611 (2000)