

# Chapter 3

## The Gross-Pitaevskii equation

### Learning goals

- What is the scattering cross-section?
- How to describe the interaction between many atoms with a mean field potential.
- Derivation and discussion of the Gross-Pitaevskii equation.
- What is the Thomas-Fermi approximation?

### 3.1 Overview

So far we have looked at the interactions between two individual particles and found that – for low energies – the scattering properties can be described by a single number, the scattering length  $a$ . The effective potential in this problem was then reduced to the pseudo potential  $V_{\text{pseudo}} = \frac{4\pi\hbar^2 a}{m}\delta(\mathbf{r})$ . This forms the basis of this chapter in which we aim to describe the interaction between all particles in a Bose-Einstein condensate. After a short introduction to the influence of quantum statistics onto the scattering cross section we move to the formulation of an effective potential, the mean field potential, formed due to the presence of many atoms. To describe the resulting wave function of a BEC we derive the Gross-Pitaevskii equation and make an important simplification, taking the Thomas-Fermi limit.

This chapter is based on the Varenna lectures of Jean Dalibard (Collisional dynamics of ultracold atomic gases, 1998), on the Les Houches lectures of Yvan Castin (Bose-Einstein condensates in atomic gases: simple theoretical results, 1999), [arXiv:cond-mat/0105058](https://arxiv.org/abs/cond-mat/0105058), and on the book Advances in Atomic Physics by C. Cohen-Tannoudji and D. Guery-Odelin.

### 3.2 Scattering cross section

The scattering amplitude  $f(\mathbf{k}, \mathbf{r})$  can be used to define a scattering cross section. For a spherically symmetric scattering potential,  $V(\mathbf{r}) = V(r)$ , one can write  $f(\mathbf{k}, \mathbf{r}) \rightarrow f(k, \Theta)$ . The differential scattering cross section, defined as the probability to find a scattered particle in the solid angle  $d\Omega$  is then

$$\frac{d\sigma}{d\Omega} = |f(k, \Theta)|^2. \quad (3.1)$$

Integration over  $\int d\Omega$  yields the total scattering cross section which – again taking the limit of very low energies as in the previous chapter – only depends on the scattering length  $a$ ,

$$\sigma_{\text{tot}} \stackrel{k \rightarrow 0}{=} 4\pi a^2. \quad (3.2)$$

We so far considered the scattering of distinguishable particles. This allows us to distinguish between the two situations shown in Figure 3.1, where the scattering amplitude is given by

either  $f(k, \Theta)$ , or by  $f(k, \pi - \Theta)$ . The situation changes if we now consider indistinguishable particles. As shown in the two scattering diagrams, the two corresponding scattering amplitudes can not be distinguished any more because the wave packets overlap in the scattering region. The two-body wave functions have to be either symmetric (bosons) or antisymmetric (fermions), and the resulting scattering amplitude thus has to be rewritten as  $f(\Theta) \pm f(\pi - \Theta)$ , for bosons (+) respectively for fermions (-). As consequence, the differential scattering cross sections and total cross sections become (again in the limit  $k \rightarrow 0$ )

$$\frac{d\sigma}{d\Omega} = |f(\Theta) \pm f(\pi - \Theta)|^2 \xrightarrow{\int d\Omega} \begin{cases} \sigma_{\text{bosons}} &= 8\pi a^2 \\ \sigma_{\text{fermions}} &= 0 \end{cases}, \quad (3.3)$$

where the integral has to be carried out only in the interval  $\Theta \in [0, \pi/2[$  in order not to overcount terms.

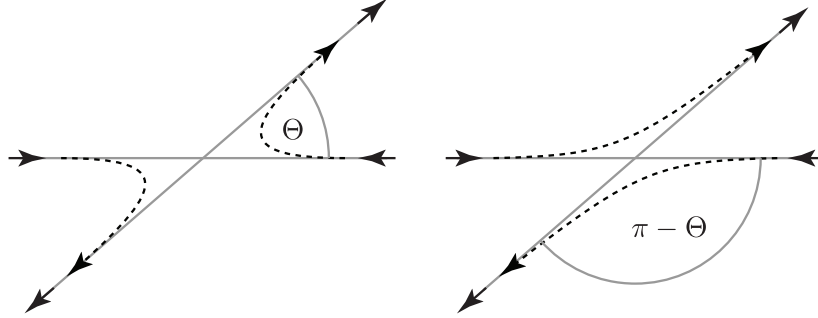


Figure 3.1: **Scattering of indistinguishable particles.** The two possible ways in which two indistinguishable particles can scatter lead to the final state. The scattering amplitudes have to be added according to the quantum statistics of the particles.

This is a remarkable result: The scattering of indistinguishable bosons is enhanced with respect to the classical case, while the scattering of fermions is completely suppressed in the limit of very low energies. As a consequence, the evaporative cooling of a spin polarized fermionic gas is impossible and different experimental techniques have to be applied.

### 3.3 Mean-field energy and effective refractive index

How can the interactions in a BEC be theoretically modeled? A starting point is to consider the change in the wave function of a single particle due to its collisions with other particles. For this discussion we assume to be in the dilute limit, where the inter-particle distance is always much larger than the scattering length,  $n|a|^3 \ll 1$ , and we assume that the gas is at ultralow temperatures, such that all scattering properties can be cast into the scattering length  $a$  (i.e. only s-wave scattering takes place). As shown in Fig. 3.2, we consider a particle with position  $\mathbf{r}_p$  and momentum  $\hbar\mathbf{k}_p = \hat{z}k_p$  traveling along the  $z$ -direction. At  $z = 0$ , the atom enters a slab of thickness  $L$  consisting of other atoms. The scattering at a single atom inside the slab at rest ( $\mathbf{k}_1 = 0$ ) at position  $\mathbf{r}_1$  is described in relative coordinates  $\mathbf{r}$  and  $\mathbf{k}$  by

$$\psi(\mathbf{r}) \propto e^{i\mathbf{k}\mathbf{r}} - \frac{a}{r}e^{ikr}. \quad (3.4)$$

The scattering state in the laboratory frame can thus be expressed as the product of center-of-mass motion and relative motion,

$$\psi_{\text{lab}}(\mathbf{r}_p, \mathbf{r}_1) = \psi_{\text{com}}(\mathbf{r})\psi(\mathbf{r}) = e^{i\mathbf{k}_{\text{com}}\mathbf{r}_{\text{com}}} \left( e^{i\mathbf{k}\mathbf{r}} - \frac{a}{r}e^{ikr} \right) \quad (3.5)$$

$$= e^{ik_p z_p} - \frac{a}{|\mathbf{r}_p - \mathbf{r}_1|} e^{i\frac{k_p}{2}|\mathbf{r}_p - \mathbf{r}_1|} e^{i\frac{k_p}{2}(z_p + z_1)}. \quad (3.6)$$

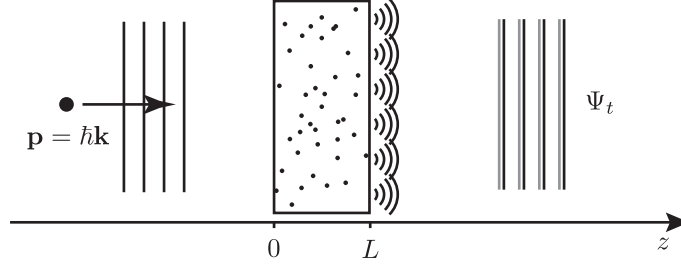


Figure 3.2: **Effective index of refraction.** A particle with initial momentum  $\mathbf{p}$  is incident on a slab of atomic medium with thickness  $L$ . The transmitted wavefunction will acquire a phase shift due to the effective index of refraction.

The final scattering state after crossing the whole slab will be the superposition of the initial state and all scattered waves resulting from collisions of the incident particle with the  $N$  particles inside the slab, neglecting multiple scattering events

$$\Psi_{\text{lab}}(\mathbf{r}_p, \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = e^{ik_p z_p} - \sum_{j=1}^N \frac{a}{|\mathbf{r}_p - \mathbf{r}_j|} e^{i\frac{k_p}{2}|\mathbf{r}_p - \mathbf{r}_j|} e^{i\frac{k_p}{2}(z_p + z_j)}. \quad (3.7)$$

To find the transmitted wave  $\psi_T(z_p)$ , we project this state onto the subspace where all scatterers are still at rest. We convert the sum into an integral  $n \int d^3r$ , use cylindrical coordinates along the  $z$ -axis with origin at  $\mathbf{r}_p$ , and find at first order in the density (details see Feynman lectures I, 30.7 - light scattering)

$$\psi_T(z_p) = \left(1 - i\frac{4\pi a n L}{k_p}\right) e^{ik_p z_p} \approx e^{-i4\pi a n L/k_p} e^{ik_p z_p}, \quad (3.8)$$

where the last transformation can be made in the limit of a thin slab. We see that the incoming wave simply acquires a phase shift while passing the slab, which thus acts as a medium with an effective index of refraction. The phase shift corresponds to a change of the wavevector inside the slab by

$$\delta k_p = -\frac{4\pi a n}{k_p}, \quad (3.9)$$

which can also be expressed as a change in kinetic energy inside the slab

$$\Delta E_{\text{kin}} = \frac{\partial E_{\text{kin}}}{\partial k} \delta k_p = -\frac{4\pi \hbar^2 a n}{m}. \quad (3.10)$$

This corresponds to a potential  $U$  which the particle experiences inside the slab:

$$U = \frac{4\pi \hbar^2 a n}{m}. \quad (3.11)$$

We here obviously again found the strength of the pseudo potential  $V_{\text{pseudo}}(\mathbf{r}) = U_0 \delta(\mathbf{r}) = \frac{4\pi \hbar^2 a}{m} \delta(\mathbf{r})$  for the interaction between two particles from last lecture, now multiplied by the density for the case of many atoms.

### 3.4 The Gross-Pitaevskii equation

For a fully condensed system, all particles are in the same single particle state  $\phi(\mathbf{r})$  with  $\int d^3r |\phi(\mathbf{r})|^2 = 1$ . The wave function describing the condensate in a mean field (or Hartree) approach is the symmetrized product of single-particle wave functions,

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \Pi_{i=1}^N \phi(\mathbf{r}_i). \quad (3.12)$$

This wave function will be influenced by the kinetic energy, the potential energy and the interaction energy. The latter is taken into account via the mean field energy  $U_0 = \frac{4\pi\hbar^2 a}{m}$  which  $(N - 1)$  particles create for one. The corresponding Hamiltonian then reads

$$H = \sum_{i=1}^N \left( \frac{\mathbf{p}_i^2}{2m} + V(\mathbf{r}_i) \right) + U_0 \sum_{i < j} \delta(\mathbf{r}_i - \mathbf{r}_j). \quad (3.13)$$

Using this Hamiltonian to find the according wave function of the BEC is a very hard problem. Instead, we can make use of a variational approach. We assume the condensate wavefunction to be  $\psi(\mathbf{r}) = \sqrt{N}\phi(\mathbf{r})$ , and the according particle density to be  $n(\mathbf{r}) = |\psi(\mathbf{r})|^2$ . Neglecting terms on the order of  $1/N$  which is save for large atom numbers, the energy functional for the  $N$ -particle wave function is given by

$$E(\phi, \phi^*) = N \int d^3\mathbf{r} \left( \frac{\hbar^2}{2m} |\nabla\phi(\mathbf{r})|^2 + V(\mathbf{r})|\phi(\mathbf{r})|^2 + \frac{1}{2}NU_0|\phi(\mathbf{r})|^4 \right) \quad (3.14)$$

A solution for the wave function can now be found by minimizing this energy functional under variations of  $\phi$  with the constraint  $\int d^3\mathbf{r}|\phi(\mathbf{r})|^2 = 1$ , i.e. that the total number of atoms stays constant. The calculus can be carried out with the help of a Lagrange multiplier  $\mu$ :

$$X(\phi, \phi^*) = E(\phi, \phi^*) - \mu N \int d^3\mathbf{r}|\phi(\mathbf{r})|^2. \quad (3.15)$$

We now need to find the minimum in the variation of  $X$ , i.e.  $\delta X = 0$ , due to variations of the wave function  $\phi \rightarrow \phi + \delta\phi$ . We find for  $\delta X$ <sup>1</sup>

$$\delta X = N \int d^3\mathbf{r} \left( \frac{\hbar^2}{2m} \nabla\phi\nabla\delta\phi^* + V(\mathbf{r})\phi\delta\phi^* + NU_0|\phi|^2\phi\delta\phi^* - \mu\phi\delta\phi^* \right) + c.c. \quad (3.16)$$

The wave function will have an imaginary and a real part. The variations in both parts should be regarded as independent, which means that  $\delta X$  has to vanish independently for  $\delta\phi$  and  $\delta\phi^*$ . We thus find<sup>2</sup>

$$\boxed{\left( -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + U_0|\psi(\mathbf{r})|^2 \right) \psi(\mathbf{r}) = \mu\psi(\mathbf{r})}, \quad (3.17)$$

where we introduced for convenience the wave function  $\psi(\mathbf{r}) = N^{1/2}\phi(\mathbf{r})$  of the condensate. Equation (3.17) is the time-independent Gross-Pitaevskii equation (GPE). It is a type of non-linear Schrödinger equation, where the total potential consists of the external potential  $V(\mathbf{r})$  and a non-linear term  $U_0|\psi(\mathbf{r})|^2$  which describes the mean-field potential of the other atoms. The eigenvalue  $\mu$  is the chemical potential. Note that it differs from the mean energy per particle  $E/N$  as it would be found for a linear equation.

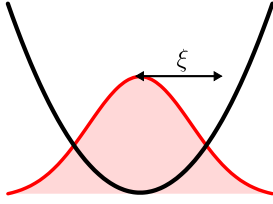
If we consider a homogeneous, interacting gas, the GPE reduces to  $U_0|\psi(\mathbf{r})|^2 = \mu$ , i.e.  $\mu = nU_0$ . This result can also be found using the thermodynamic relation  $\mu = \partial E / \partial N$  with  $E = U_0/V \cdot N(N - 1)/2 \approx U_0/V \cdot N^2/V$ .

### 3.5 The Thomas-Fermi approximation

We have seen that the full many-particle system can be reduced to the problem of finding a single particle, or condensate, wave function. The Gross-Pitaevskii equation determines the shape of this wave function. While being a tremendous simplification with respect to the original problem, it is still a *non-linear* Schrödinger equation to which we have generically no exact solution. In this section we learn how to simplify the full Gross-Pitaevskii equation in the presence of a trap.

<sup>1</sup>using  $\nabla(\phi + \delta\phi)\nabla(\phi^* + \delta\phi^*) = |\nabla\phi|^2 + \nabla\phi\nabla\delta\phi^* + \nabla\phi^*\nabla\delta\phi + \nabla\delta\phi\nabla\delta\phi^*$  and  $(\phi + \delta\phi)\phi^* + \delta\phi^* = |\phi|^2 + \phi\delta\phi^* + \phi^*\delta\phi + \delta\phi\delta\phi^*$  and using only terms linear in the variations  $\delta\phi$ .

<sup>2</sup>We first apply a partial integration of the kinetic energy to get the same expression  $\phi\delta\phi^*$  as in the other terms. Then we set the full integrant to zero.



The equation we try to solve is given by

$$\mu\psi(\mathbf{r}) = \left[ -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + U_0|\psi(\mathbf{r})|^2 \right] \psi(\mathbf{r}). \quad (3.18)$$

Let us consider a harmonic potential

$$V(\mathbf{r}) = \frac{m\omega_0^2}{2}r^2. \quad (3.19)$$

By assuming a cloud of size  $\xi$  we can estimate both the average kinetic as well as the average potential energy per particle

$$\bar{E}_{\text{kin}} \sim \frac{\hbar^2}{2m\xi^2}, \quad (3.20)$$

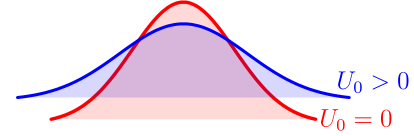
$$\bar{V} \sim \frac{m\omega_0^2}{2}\xi^2. \quad (3.21)$$

Owing to the virial theorem we can equate the two to find the typical cloud size for  $U_0 = 0$

$$\xi = \sqrt{\frac{\hbar}{m\omega_0}}. \quad (3.22)$$

Of course we would have obtained the same radius by solving the harmonic oscillator problem for  $\psi(\mathbf{r})$  given that  $U_0 = 0$ .

Let us now consider the influence of the interaction energy assuming that we have a typical particle density  $n = N/\xi^3$ , where  $N$  denotes the number of particles. We find for the average interaction energy per particle



$$\bar{E}_{\text{int}} \sim U_0 n \sim U_0 \frac{N}{\xi^3}. \quad (3.23)$$

Comparing this to the estimate of the kinetic energy (3.20) we see that in a trap, both the interaction as well as the kinetic energy work in the same direction, i.e., both try to expand the cloud! Owing to this we can try to neglect the weaker of the two without picking up too much of an error. If we compare kinetic and interaction energies we see that if  $U_0$  exceeds the critical strength

$$U_0^{\text{crit}} \sim \frac{\hbar\omega_0}{2n} \quad (3.24)$$

we can neglect the kinetic term. This approximation is called the *Thomas-Fermi approximation*.<sup>3</sup> Using the Thomas-Fermi approximation we can estimate the typical cloud size in the presence of interaction  $R$

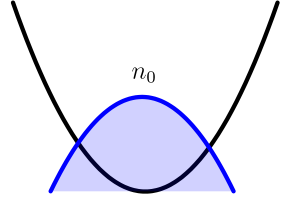
$$\partial_R \left( \frac{m\omega_0^2}{2}R^2 + U_0 \frac{N}{R^3} \right) = m\omega_0^2 R - 3U_0 N \frac{1}{R^4} \stackrel{!}{=} 0. \quad (3.25)$$

Therefore we obtain

$$R \sim \left( \frac{NU_0}{m\omega_0^2} \right)^{1/5} \sim \xi \left( \frac{Na}{\xi} \right)^{1/5}, \quad (3.26)$$

<sup>3</sup>The fact that both work in the same direction is absolutely essential in this step. Remember that the Gross-Pitaevskii equation is based on *weak interactions*. If the effect of interactions would oppose the one of the kinetic energy, we could not skip the latter without violating the underlying assumption of weak interactions.

where we replaced the interaction constant  $U_0 = 4\pi\hbar^2 a/m$  with the scattering length  $a$  to highlight how the non-interacting cloud size is changed by another length scale  $Na$ . Moreover, if we can solve the Gross-Pitaevskii equation in the Thomas-Fermi limit exactly. It is straight forward to check that



$$n(\mathbf{r}) = |\psi(\mathbf{r})|^2 = \begin{cases} \frac{\mu - V(\mathbf{r})}{U_0} & \text{for } \mathbf{r} \text{ such that } \frac{\mu - V(\mathbf{r})}{U_0} > 0, \\ 0 & \text{otherwise,} \end{cases} \quad (3.27)$$

indeed is a solution of  $\mu\psi = (U_0|\psi|^2 + V)\psi$ . Using the normalization condition  $\int d\mathbf{r} n(\mathbf{r}) = 1$  we find the chemical potential  $\mu$ , or more interestingly the density in the center of the trap  $n_0$

$$R^2 = \frac{2\mu}{m\omega_0^2} \Rightarrow N = \left( \frac{2\mu}{m\omega_0^2} \right)^{3/2} \frac{\mu}{U_0} \Rightarrow \mu \sim N^{2/5} \quad \text{and hence} \quad n_0 \sim N^{2/5}. \quad (3.28)$$