Markus Holzmann LPMMC, Maison de Magistère, Grenoble, and LPTMC, Jussieu, Paris markus@lptl.jussieu.fr http://www.lptl.jussieu.fr/users/markus (Dated: May 18, 2012)

We will consider the very basic properties of dilute Bose gases in homogeneous and trapped systems. We remind the basic results of scattering theory, and argue that the interaction of quantum gases at low temperatures is well described by the first phase shifts, in many cases, via the s-wave scattering length only. There are various formalisms to account for that, here we use a simple zero-range pseudo-potential. The Hartree ansatz for the wavefunction leads directly to the Gross-Pitaevskii equation for the condensate at zero temperature. We will derive the finite-temperature mean-field equation and the Bose-Einstein transition in mean-field by using minimizing a variational upper bound for the free energy.

We will look at the problem of interacting Bosons, mainly with the aim to describe the experimens of Bose-Einstein condensation of alcaline atoms in trapped systems. Some time will be spend with the two-body problem. Many properties of Bose condensates can be quantitatively explained by a simple non-linear Schrödinger equation, the Gross-Pitaevskii equation. However, in the non-linearity enters the scattering length, and not the bare potential. For analytical calculations, zero-range pseudo-potentials are quite useful.

A. Interacting Bosons: the two-body problem

In order to understand the N-body problem, we need some basic concepts and results from quantum scattering theory concerning simple two-body collisions. Quite generally, we can assume that the interaction potential between two particles, $V(\mathbf{r}_1, \mathbf{r}_2) = V(|\mathbf{r}|)$, depends only on the relative coordinate, $\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2$. We further assume, that the external potential also seperates in relative, and center-of-mass coordinates, so that the complete Hamiltonian of the two particles writes

$$H_{12} = H_{cm} + H_0 + V(|\mathbf{r}|) \tag{1}$$

$$H_0 = \frac{\hbar^2}{2m_r} \Delta_{\mathbf{r}} \tag{2}$$

where $m_r = m/2$ and H_{cm} depends only on the center-of-mass coordinates $\mathbf{r}_{cm} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, e.g. a homogeneous system, or a system in an external harmonic potential. The wavefunction therefore separates

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_{cm}(\mathbf{r}_{cm})\phi(\mathbf{r}) \tag{3}$$

and we will concentrate on $\phi(\mathbf{r})$ in the following, which contains all collisional properties and is determined by

$$(H_0 + V)|\phi\rangle = E|\phi\rangle \tag{4}$$

together with the boundary conditions on $|\phi\rangle$.

For a formal solution, we rearrange the Schrödinger equation

$$|E - H_0|\phi\rangle = V|\phi\rangle \tag{5}$$

Starting from the known free solution, $|\phi_0(E)\rangle$, which satisfies the homogeneous equation,

$$(E - H_0)|\phi_0\rangle = 0\tag{6}$$

we would like to obtain the full solution of Eq. (5) by inverting the operator $E - H_0$. However, since for a continuous, infinite system, scattering states will have the same energy than the free states, we cannot invert $(E - H_0)^{-1}$, but we introduce a small imaginary offset

$$|\phi^{\pm}(E)\rangle = |\phi_0(E)\rangle + \frac{1}{E - H_0 \pm i\epsilon} V |\phi^{\pm}(E)\rangle$$
(7)

with infinitesimal $\epsilon > 0$. As we will see, the wave functions ϕ^{\pm} describe different sets of solutions. Eq. (7) is called Lippmann-Schwinger equation.

1. Scattering amplitude and cross section

The interatomic (or molecular) potential is not necessarily known with high precision. Therefore, theoretical results on the N-particle problem should be expressed in terms of measurable quantities. Here we analyse the scattering problem in terms of quantities which may be obtained directly from scattering experiments, e.g the scattering amplitude and the cross section.

Let us start analyzing the Lippmann-Schwinger equation, Eq. (7), in position space, using plane waves.

$$\phi_{\mathbf{k}}^{\pm}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \int d^{3}\mathbf{r}' G^{\pm}(\mathbf{r} - \mathbf{r}'; E = k^{2}/2m_{r})V(r')\phi_{\mathbf{k}}^{\pm}(\mathbf{r}')$$
(8)

where

$$G^{\pm}(\mathbf{r} - \mathbf{r}'; E) = \langle \mathbf{r} | \frac{1}{E - H_0 \pm i\epsilon} | \mathbf{r}' \rangle$$
(9)

Explicitly, in three dimensions, d = 3, we have

$$G^{\pm}(\mathbf{r} - \mathbf{r}'; E) = \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot(\mathbf{r} - \mathbf{r}')} \frac{2m_r}{2m_r E - q^2 \pm i\epsilon} = \frac{2m_r}{(2\pi)^2} \int_0^\infty dq \, \frac{q^2}{2m_r E - q^2 \pm i\epsilon} \frac{e^{iq|\mathbf{r} - \mathbf{r}'|} - e^{-iq|\mathbf{r} - \mathbf{r}'|}}{iq|\mathbf{r} - \mathbf{r}'|} \tag{10}$$

$$=\frac{2m_r}{(2\pi)^2}\frac{1}{i|\mathbf{r}-\mathbf{r}'|}\int_{-\infty}^{\infty}dq\,\frac{qe^{iqr}}{(\sqrt{2m_rE}-q)(\sqrt{2m_rE}+q)\pm i\epsilon}=-\frac{2m_r}{4\pi}\frac{e^{\pm i\sqrt{2m_rE}|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}\tag{11}$$

Inserting into Eq. (8), we get

$$\Psi_{\mathbf{k}}^{\pm}(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k}',\mathbf{k};k^2/2m_r\pm i\epsilon)\frac{e^{\pm ikr}}{r}, \quad \text{large } r \text{ with } \mathbf{k}' \equiv k \mathbf{r}/r$$
(12)

$$f(\mathbf{k}', \mathbf{k}; E = k^2 / 2m_r \pm i\epsilon) = -\frac{2m_r}{4\pi} \int d\mathbf{r}' e^{-i\mathbf{k}' \cdot \mathbf{r}'} V(r') \Psi_{\mathbf{k}}^{\pm}(\mathbf{r}'), \qquad (13)$$

Using the asymptotic solution $\Psi_{\mathbf{k}}^{+}(\mathbf{r})$ in Eq. (12), we describe the scattering of an incident plane wave of wave vector \mathbf{k} with a scattered outgoing spherical wave of amplitude $f(\mathbf{k}', \mathbf{k}; E = k^2/2m_r + i\epsilon)$ where \mathbf{k}' points into the scattering direction. The flux of of scattered particles into direction \mathbf{k}' is then proportional to the square of the scattering amplitude, and the differential cross section writes

$$\frac{d\sigma}{d\Omega} = |f(\mathbf{k}', \mathbf{k}; E = k^2/2m_r + i\epsilon)|^2 \tag{14}$$

2. Partial wave analysis

For a detailed analysis of the scattering problem including explicit solutions, it is useful to adapt to the symmetry of the problem. Using rotational symmetry, we introduce angular coordinates (r, θ, φ) and we separate the angular part of the wavefunction using the eigenfunctions of angular momentum

$$\phi(\mathbf{r}) = \sum_{nlm} a_{nml} \frac{u_{nl}(r)}{r} Y_{lm}(\theta, \varphi)$$
(15)

where the spherical harmonics $Y_{lm}(\theta, \varphi) \propto P_l(\cos \theta) e^{im\varphi}$ can be expressed using the Legendre polynomials $P_l(x)$. Since $|\mathbf{k}| = |\mathbf{k}'|$ in Eq. (13), we expand the scattering amplitude only depends on the angle θ between \mathbf{k} and $\mathbf{k}' = k\mathbf{r}/r$,

$$f(\mathbf{k}', \mathbf{k}; k^2/2m_r + i\epsilon) = \sum_l (2l+1)f_l(k)P_l(\cos\theta)$$
(16)

Using now the asymptotic expansion of the plane wave in terms of spherical waves

$$e^{ikr\cos\theta} \sim \frac{1}{2ikr} \sum_{l} (2l+1)P_l(\cos\theta) \left[e^{-il\pi} e^{-ikr} + e^{ikr} \right], \quad kr \gg 1$$
(17)

we get from Eq. (12) and Eq. (15) (with n = k in the infinite system limit)

$$u_{kl}(r) \sim \frac{1}{2ikr} \sum_{l} (2l+1)P_l(\cos\theta) \left[e^{-il\pi} e^{-ikr} + [1+2ikf_l(k)]e^{ikr} \right], \quad kr \gg 1$$
(18)

Due to flux conservation in each partial wave, the absolute value of the amplitude of in-going waves e^{-ikr} must equal that of out-going waves e^{ikr} so that $[1+2ikf_l(k)] = e^{i2\delta_l(k)}$ with real $\delta_l(k)$. The total scattering amplitude then writes

$$f(\mathbf{k}', \mathbf{k}; k^2/2m_r + i\epsilon) = \frac{1}{2ik} \sum_l (2l+1) \left[e^{2i\delta_l(k)} - 1 \right] P_l(\cos\theta)$$
(19)

in terms of the phase shifts, $\delta_l(k)$, and the radial wave function is asymptotically given by

$$u_{kl}(r) \sim \frac{1}{2ikr} \sum_{l} (2l+1)P_l(\cos\theta) \left[e^{-il\pi} e^{-ikr} + e^{i2\delta_l(k)} e^{ikr} \right] \sim e^{-i(l\pi/2 - \delta_l(k))} \sin\left[kr - l\pi/2 + \delta_l(k)\right]$$
(20)

3. Low energy scattering

Phase shifts for a given potential can be obtained by directly solving the Schrödinger equation using partial waves in a spherical box of infinite radius. The radial part satisfies a one-dimensional differential equation for each angular momentum l

$$-\frac{\hbar^2}{2m_r}\frac{d^2u_{nl}(r)}{dr^2} + \left[\frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right]u_{nl}(r) = E_{nl}u_{nl}(r)$$
(21)

The interatomic potential V has a characteristic length scale R_e ; for distances $r > R_e$ we can neglect the potential, $V(r > R_e) \equiv 0$. For vanishing potential corresponding to free particles, the solution of Eq. (21) are the spherical Bessel functions, $j_l(kr)$ and $n_l(kr)$, with $k = \sqrt{2m_r E_{nl}/\hbar^2}$. The solution of Eq. (21) for $r < R_e$ has to be calculated for any specific potential V(r) and can then be matched at $r = R_e$ to the free solution, such that the wavefunction and its derivative are continuous functions at $r = R_e$. The outside solution is a superposition of j_l and n_l which is conviniently written as

$$\frac{u_l(kr)}{kr} \equiv \frac{u_{nl}(r)}{kr} = 2\left[\cos\delta_l j_l(kr) - \sin\delta_l n_l(kr)\right]$$
(22)

Writing the superposition coefficient in terms of the phase shift $\delta_l(k)$ is motivated by considering the large distance asymptotic of the Bessel functions

$$j_l(x) \to \frac{\sin\left[x - l\frac{\pi}{2}\right]}{x}, \quad x \to \infty$$
 (23)

$$n_l(x) \rightarrow -\frac{\cos\left[x - l\frac{\pi}{2}\right]}{x}, \quad x \to \infty$$
 (24)

so that we get

$$\frac{u_l(kr)}{kr} \to 2 \frac{\sin\left[kr - l\frac{\pi}{2} + \delta_l\right]}{kr} \approx 2j_l(kr + \delta_l), \quad kr \to \infty$$
⁽²⁵⁾

Hard sphere scattering. Note that for small arguments, the Bessel functions behave as

$$j_l(x) \rightarrow \frac{x^l}{(2l+1)!!}, \quad x \rightarrow 0$$

$$(26)$$

$$n_l(x) \to -\frac{(2l-1)!!}{x^{l+1}}, \quad x \to 0$$
 (27)

For hard spheres, the wavefunction has to vanish at r = a where a is the diameter of one sphere, or $u_l(ka) \equiv 0$. Using the asymptotic expansion (27), valid for low-energy scattering, in the expression (22), we obtain for the phase-shift

$$\tan \delta_l \simeq -\frac{(ka)^{2l+1}}{(2l+1)!!(2l-1)!!}, \quad ka \to 0$$
⁽²⁸⁾

In this low energy limit $ka \to 0$, the dominant contribution comes from l = 0, called s-wave scattering. Note that the s-wave phase shift $\delta_0 = -ka$ is negative for the repulsive potential.

Scattering length, alcaline atoms. For low-energy scattering $(k \rightarrow 0)$ one introduces the s-wave scattering length a_s for a general interaction potential writing

$$\frac{k}{\tan \delta_0} = -\frac{1}{a_s} + \frac{1}{2}r_{eff}k^2$$
(29)

where r_{eff} is called effective range of the potential. The phase shift, and therefore also the scattering length can be measured. Let us consider alcaline atoms. The short range interactions at the range of the Bohr radius is dominated by the exchange energies of the overlapping electronic wavefunctions, and strongly repulsive. The long-range tail of the interaction can be described by a van-der-Waals interaction $V(r) = -C_6/r^6$ with characteristic distance $R_e = (4mC_6/\hbar^2)^{1/4}$ with $\hbar^2/(2\mu R_e^2) = C_6/R_e^6$. For alcalines R_e ranges from 20 Å for Li, 80 Å for Rb, up to 100 Å for Cs. For larger distances, the scattering properties are described by the phase shifts, corresponding to a scattering length of 55 Å for Rb, and -600 Å for Cs.

4. Universality and pseudo-potentials

If we consider properties where the distance between partiicles is large compared to the characteristic length scale of the interaction R_e , we expect that we can express all properties by the phase shifts. The properties which depend only on the phase shifts are universal with respect to different interactions. Since we can obtain the same phase-shifts for different microscopic interactions, we are free to choose the one which is best suited for our calculations. These potentials are called pseudo-potentials. In particular, at low energy, we generally have

$$f(\mathbf{k}, \mathbf{k}'; k^2/2m_r + i\epsilon) = -a_s, \quad k \to 0$$
(30)

and the scattering amplitude is minus the scattering length which is the only parameter needed to describe collisions.

The idea of pseudo-potentials is to replace the true scattering potentials by a model. The model is chosen to simplify the calculations still maintaining the scattering properties.

A particular simple potential for analytical calculations would be a delta-function potential $g\delta(\mathbf{r})$. However, inserting it together with Eq. (12) (continued to $\mathbf{r} = 0$) in Eq. (13), we get $f = -2m_rg/4\pi \lim_{r\to 0} [1 + f/r]$. As long as we would restrict to first order in $f \sim g$, we get a simple result, but the second order is diverging. Note that the small corrections in r'^2/r^2 neglected in Eq. (12) to describe the full behavior outside the scattering potential do not change this result.

Since, the simple delta-function potential cannot be used in general, a regularized delta-function potential eliminates this problem

$$\tilde{V}_{\delta}(\mathbf{r}) = g\delta(\mathbf{r}) \left[\frac{d}{dr} r \cdot \right]$$
(31)

The scattering amplitude, Eq. (13), is now given by

$$f(\mathbf{k}', \mathbf{k}; E = k^2 / 2m_r + i\epsilon) = -\frac{2m_r}{4\pi} \int d\mathbf{r}' e^{-i\mathbf{k}' \cdot \mathbf{r}'} V_{\delta}(r') \Psi_{\mathbf{k}}^+(\mathbf{r}') = -\frac{2m_r g}{4\pi} \lim_{r \to 0} \frac{d}{dr} \left(r \Psi_{\mathbf{k}}^+(r) \right)$$
(32)

which gives a close relation using Eq. (12) for $\Psi_{\mathbf{k}}^+(r \to 0)$:

$$f(\mathbf{k}', \mathbf{k}; E = k^2/2m_r + i\epsilon) = -\frac{2m_r g}{4\pi} \frac{1}{1 + ik2m_r g/4\pi}$$
(33)

In order to recover the scattering length for vanishing momenta, we set $g = 4\pi a/2m_r$ and get

$$f(\mathbf{k}', \mathbf{k}; E = k^2/2m_r + i\epsilon) = -\frac{a}{1+ika}$$
(34)

Note that acting with the regularized pseudopotentials, Eq. (31) on functions which are regular at the origin, reduces to the action of a simple delta-function potential.

The exact solution of the two-body wave function for the regularized pseudo-potential is

$$\Psi_{\mathbf{k}}^{+}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{a}{1+ika} \frac{e^{\pm ikr}}{r}$$
(35)

Let us explicitly verify that Eq. (35) is indeed a solution of the Schrödinger equation. Using that

$$\Delta \frac{f(r)}{r} = \Delta \frac{1}{r} + \Delta \frac{f(r) - 1}{r} = 4\pi \delta(\mathbf{r}) + \frac{f''(r)}{r}$$
(36)

for any radial function f(r) and the laplacian in d = 3, we have

$$-\Delta \Psi_{\mathbf{k}}^{+}(\mathbf{r}) = k^{2} \Psi_{\mathbf{k}}^{+}(\mathbf{r}) + \frac{4\pi a}{1 + ika} \delta(\mathbf{r})$$
(37)

We then get

$$\left[-\Delta + 2m_r\hbar^{-2}V_{\delta}(\mathbf{r})\right]\Psi_{\mathbf{k}}^{+}(\mathbf{r}) = k^2\Psi_{\mathbf{k}}^{+}(\mathbf{r}) + \frac{4\pi a}{1+ika}\delta(\mathbf{r}) + 2m_r\hbar^{-2}g\delta(\mathbf{r})\left[1 - \frac{iak}{1+ika}\right] = k^2\Psi_{\mathbf{k}}^{+}(\mathbf{r})$$
(38)

so that $\Psi_{\mathbf{k}}^{+}(\mathbf{r})$ is an energy-eigenfunction with energy $k^{2}/2m_{r}$. Since we expect that also the N-body wave function of a gas must be an eigenfunction of the two-body Hamiltonian for two particles coming arbitrary close to each other, the wave function must be proportional to Eq. (35) when all the other N-2 particles are kept fixed. At low temperatures, we can use the limit $k \to 0$ and we get

$$\Psi_N(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \to (1 - a/|\mathbf{r}_i - \mathbf{r}_j|) \tilde{\Psi}_{ij}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N), \quad \text{for any } \mathbf{r}_i \to \mathbf{r}_j$$
(39)

where $\tilde{\Psi}_{ij}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ is regular when $\mathbf{r}_i \to \mathbf{r}_j$. Notice that the wave function is well defined for all $|\mathbf{r}_i - \mathbf{r}_j|$, including distances smaller than a, so that the a/r in the wave function will dominate the momentum distribution at large k, leading to an universal behavior.

Delta-Potential truncated in momentum space 5.

Perturbation expansions of the many-body problem are often done in Fourier-space, and the application of the real-space pseudopotential is not always simple there. In this case, we can define a smooth potential by

$$V_{\eta}(\mathbf{k}) = \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} V(r) = g_0 \eta(k)$$
(40)

with $\eta(k) = 1$ for $k \ll k_c$ and $\eta(k) = 0$ for $k \gg k_c$. The true delta function would be described by $k_c \to \infty$, but this will introduce divergent expressions, circumvented by the use of a large, but finite k_c .

Let us look directly at the T-matrix given by

$$T_{\mathbf{k},\mathbf{k}'} = \langle \mathbf{k} | V | \Psi_{\mathbf{k}'}^+ \rangle \tag{41}$$

which can be generalized inserting the Lippmann-Schwinger equation, Eq. (7), to obtain the operator equation (for general E)

$$T(E) = V + V \frac{1}{E - H_0 + i\epsilon} T(E)$$

$$\tag{42}$$

Note the connection to the scattering amplitude, Eq. (13),

$$\langle \mathbf{k} | T(E = k^2/2m + i\epsilon) | \mathbf{k}' \rangle = -\frac{4\pi}{2m_r} f(\mathbf{k}, \mathbf{k}'; k^2/2m_r + i\epsilon)$$
(43)

We then have for our model potential

$$T_{\mathbf{k}\mathbf{k}'}(E) = g_0 \eta(\mathbf{k} - \mathbf{k}') + \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{g_0 \eta(\mathbf{k} - \mathbf{q})}{E - q^2/2m_r + i\epsilon} T_{\mathbf{q}\mathbf{k}'}(E)$$
(44)

For E around $k^2/2m_r$ we can approximate $T_{\mathbf{qk}'}(E) \approx T_{\mathbf{kk}'}(E)$ since the nominator is peaked around $q \approx k$. We then get

$$T_{\mathbf{k}\mathbf{k}'}(E) = g_0 \eta(\mathbf{k} - \mathbf{k}') + T_{\mathbf{k}\mathbf{k}'}(E) \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{g_0 \eta(\mathbf{k} - \mathbf{q})}{E - q^2/2m_r + i\epsilon}$$
(45)

or

$$T_{\mathbf{k}\mathbf{k}'}(E) = \frac{g_0\eta(\mathbf{k} - \mathbf{k}')}{1 + g_0 \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{\eta(\mathbf{k} - \mathbf{q})}{E - q^2/2m_r + i\epsilon}}$$
(46)

Let us now look at low energy properties, $E \sim k^2/2m_r \approx 0$, and relate the on-shell T-matrix with the scattering amplitude, Eq. (43), and using the pseudo-potential expression for s-wave scattering, we have

$$T_{\mathbf{k}\mathbf{k}'}(E = k^2/2m_r) = \frac{4\pi a}{2m_r} \frac{1}{1 + ika}$$
(47)

so that we can eliminate g_0 in favour of a, e.g. from Eq. (45) for $E \sim k^2/2m \to 0$, which we write as

$$\frac{1}{g_0} = \frac{1 + ika}{4\pi a/2m_r} - \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{\eta(\mathbf{q})}{(q^2 - k^2)/2m_r - i\epsilon}$$
(48)

We can further simplify by evaluating the integral on the rhs

$$\int \frac{d\mathbf{q}}{(2\pi)^3} \frac{\eta(\mathbf{q})}{q^2/2m_r - E - i\epsilon} = \frac{2m_r}{2\pi^2} \left[\int dq \frac{q^2 - 2m_r E}{q^2 - 2m_r E} \eta(q) - \sqrt{2m_r E} P \int dx \frac{\eta(x\sqrt{2m_r E})}{1 - x^2} + i\pi \int dq q^2 \delta(q^2 - 2m_r E) \right] \\ = \frac{2m_r}{4\pi^2} \left[Ck_c + i\frac{\pi}{2}\sqrt{2m_r E} \right]$$
(49)

where $C = \int_0^\infty d(q/kc)\eta(q/k_c)/2$ is a constant of order one. We then have

$$g = \frac{g_0}{1 + 2m_r C g_0 k_c / 4\pi} \tag{50}$$

where $g = 4\pi a/2m_r$, or

$$g_0 = \frac{g}{1 - Cak_c} \tag{51}$$

Notice that second order effects in g_0 are not proprotional to second order effects in a.

B. Ground state wavefunction for a Bose gas (T = 0): variational calculation

We are in the following considering the experiments on Bose-Einstein condensation with (metastable) alcaline atoms. Typically $N \sim 10^7$ atoms are confined in a harmonic trapping potential with typical peak densities $n \leq 10^{15} cm^{-3}$. The typical interparticle distance $n^{-1/3} \leq 10^3$ Å is large compared to the characteristic distance R_e of the van-der Waals interaction, and many low-temperature properties should be well universal in terms of the scattering length a. Further, we also have $na^3 \ll 1$ characteristic for a dilute gas.

Since the system is dilute, on might consider an ideal gas Hartree wavfunction as a first starting point for the ground state wavefunction

$$\Psi_0(\mathbf{R}) = \prod_i \varphi(\mathbf{r}_i) \tag{52}$$

and minimize the variational energy $\langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle$ to obtain the best single particle wavefunction φ . However, the real interparticle interaction between alcaline atoms is not smooth at all, it is rather diverging at distances comparable to the Bohr radius. Therefore, the variational energy of an ideal gas wavefunction using the bare interatomic potential is not giving any reasonable result; certainly it is not a good starting point, we have to consider effects of the interactions already in the lowest order. In addition, experiments on alcaline gases are not in the ground state (which is a solid), but they are metasable. In general, the variational principle gives only upper bounds for the energy of the true ground state and might lead into serious troubles when applied to high energy metastable states.

In order to avoid bound states already in the two-body scattering problem, one convientiently introduces pseudopotentials which lead to the same scattering properties but emiminate bound states. We will see that they also facilitate analytical calculations. Therefore we consider from now on the generic many-body Hamiltonian

$$H = \sum_{i} \left[-\frac{\hbar^2}{2m} \nabla_i^2 + u(\mathbf{r}_i) \right] + \sum_{i < j} v(r_{ij})$$
(53)

where u is the external potential and v is the interparticle pseudo-potential

$$v(r) = g\delta(\mathbf{r})\frac{d}{dr}(r\cdot), \quad g = \frac{4\pi\hbar^2 a}{m}$$
(54)

and we denote the s-wave scattering length a.

From the uncorrelated Hartree wavefunction, Eq. (52), we obtain an upper bound for the total free energy

$$E_0 - \mu N \le F[\varphi, \nabla \varphi] = N \int d\mathbf{r} \left[\frac{\hbar^2 |\nabla \varphi(\mathbf{r})|^2}{2m} + [u(\mathbf{r}) - \mu] |\varphi(\mathbf{r})|^2 + \frac{(N-1)g}{2} |\varphi|^4 \right]$$
(55)

We have used a partial integration, and vary the energy as a functional of φ and $\nabla \varphi$ independently using the Euler-Lagrange equations

$$\frac{\delta F}{\delta \varphi(\mathbf{r})} - \nabla \frac{\delta F}{\delta(\nabla \varphi)} = 0 \tag{56}$$

We obtain a non-linear Schrödinger equation

$$\left(-\frac{\hbar^2 \nabla^2}{2m} + u(r) + Ng|\varphi(r)|^2\right)\varphi(\mathbf{r}) = \mu\varphi(\mathbf{r})$$
(57)

Since all particles are in the same single-particle state $\varphi(\mathbf{r})$, this single particle wavefunction describes a Bose-Einstein condensate and the non-linear Schrödinger equation is called Gross-Pitaevskii equation in this context. The condensate wavefunction must be normalized to one, and the chemical potential corresponds to the mean energy per particle in the system at zero temperature. The density is given by

$$n(\mathbf{r}) = N|\varphi(\mathbf{r})|^2 \tag{58}$$

Ground state energy of the homogeneous system, healing length. The ground state wavefunction for a homogeneous system $u(r) \equiv 0$ must be constant and one immediatly gets

$$\mu = gn \tag{59}$$

The length scale, ξ associated with the interaction energy,

$$\frac{\hbar^2}{2m\xi^2} = gn \tag{60}$$

or

$$\xi = \sqrt{\frac{\hbar^2}{2mgn}} \tag{61}$$

is called healing length.

Thomas-Fermi approximation. Let us consider a very smoothly varying external potential. We can regard the system as locally homogeneous and treat the system in the local density approximation. The kinetic energy contribution corresponding to the laplacian in the Gross-Pitaevskii equation, Eq. (57), is expected to be small compared to the interaction contribution. This allows us to express the chemical potential as a functional of the local density $n(\mathbf{r})$

$$\mu[n(\mathbf{r})] = gn(\mathbf{r}) + u(\mathbf{r}) \tag{62}$$

However, for thermodynamic stability, the chemical potential must be constant in space, and we can determine the density distribution in an external trapping potential

$$n(\mathbf{r}) = \frac{1}{g} \left[\mu - u(\mathbf{r}) \right] = n(0) - \frac{1}{g} u(\mathbf{r}), \quad \mu - u(\mathbf{r}) \ge 0$$
(63)

and

$$n(\mathbf{r}) \equiv 0, \quad \mu - u(\mathbf{r}) < 0 \tag{64}$$

From the normalization we can easily calculate the total number of atims $N = \int d\mathbf{r} n(\mathbf{r})$ as a function of the chemical potential. Further, we can check, if the kinetic energy can be indeed neglected. Typically, the kinetic energy contribution changes the wavefunction at the egde and smoothes the distribution in order to obtain a density profile with continuous derivatives. The Thomas-Fermi distribution further breaks down for small systems.

Harmonic trapping potential. In most of the experiments, the atoms are trapped by a harmonic oscillator potential

$$u(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2 \tag{65}$$

with small (or even strong) asymmetric oscillator strengths. The typical length scale of the trapping potential is then given by the harmonic oscillator length, a_0 ,

$$\frac{1}{2}m\omega^2 a_0^2 = \frac{\hbar^2}{2ma_0^2} \tag{66}$$

or

$$a_0 = \sqrt{\frac{\hbar}{m\omega}} \tag{67}$$

The kinetic energy per particle is roughly $\sim \hbar^2/(2ma_0^2) \sim \hbar\omega$, whereas the interaction energy is proportial to the density gn(r). For $gn(r) \sim \mu \gg \hbar\omega$ or $\xi \ll a_0$, the Thomas-Fermi approximation is justified, and the density distribution has a typical parabolic shape. Whenever, the kinetic energy dominates, the wavefunction will be rather similar to the non-interacting gaussian, since the level-spacing of the trap is dominating.

Collective excitations, vortices. Stationary solutions of the Gross-Pitaevskii equation (57) with higher energies than the ground state correspond to collective excitations of the condensate. Solutions with non-zero angular momentum are called vortices. The centrifugal potential forces that the condensate wavefunction to vanish around the vortex core which is of size of the healing length ξ .

Stability, Bogoliubov excitations. The stability of the condensate with respect to small variations in the wavefunctions will lead to the Bogoliubov excitation spectrum in linear respons. These excitations remain occupied even at zero temperature and lead to a deplition of the condensate density of order of $(na^3)^{1/2}$.

Notice that even though the Hartree-wave function, Eq. (52), can give good estimates for the ground state energy, it is clear that it is never an eigenstate of the Hamiltonian, e.g. it does not satisfy the two-particle Schrödinger equation. Therefore, it is a-priori not clear, if the true system is really Bose condensed.

Appendix: Some results for the phase shifts

We have chosen the normalization for the radial wavefunction such that

$$\int_0^\infty dr u_l(kr) u_l(k'r) = 2\pi\delta(k-k') \tag{68}$$

in the continuum limit.

Let us denote $u_{nl}^{(0)}(r)$ the free solution of Eq. (21) for vanishing potential

$$-\frac{\hbar^2}{2\mu}\frac{d^2 u_{nl}^{(0)}(r)}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2}u_{nl}^{(0)}(r) = E_{nl}u_{nl}^{(0)}(r)$$
(69)

$$\frac{u_l^{(0)}(kr)}{kr} = 2j_l(kr) \tag{70}$$

We multiply Eq. (21) with $u_{nl}^{(0)}(r)$ from the left and subtract Eq. (69) multiplied by $u_{nl}(r)$. Integrating over r from 0 to R we obtain

$$\frac{2\mu}{\hbar^2} \int_0^R dr \, u_l^{(0)}(kr) V(r) u_l(kr) = -u_l(kR) \frac{du_l^{(0)}(kr)}{dr} \Big|_{r=R} + u_l^{(0)}(kR) \frac{du_l(kr)}{dr} \Big|_{r=R}$$
(71)

where we have integrated by parts and used that u_l and $u_l^{(0)}$ vanish at r = 0. For large R we can use the asymptotic expressions and obtain

$$u_{l}(kR)\frac{du_{l}^{(0)}(kr)}{dr}\Big|_{r=R} - u_{l}^{(0)}(kR)\frac{du_{l}(kr)}{dr}\Big|_{r=R} = -4k\sin\left(kr - l\frac{\pi}{2} + \delta_{l}\right)\cos\left(kr - l\frac{\pi}{2}\right) + 4k\sin\left(kr - l\frac{\pi}{2}\right)\cos\left(kr - l\frac{\pi}{2} + \delta_{l}\right) = -4k\sin\delta_{l}$$
(72)

We obtain a quite useful result

$$\int d\mathbf{r} \frac{u_l^{(0)}(rk)}{2kr} V(r) \frac{u_l(rk)}{2kr} = -\frac{4\pi\hbar^2}{m} \frac{\sin\delta_l}{k}$$
(73)