EMA601: Quantum Engineering with Atoms and Photons
University of Wisconsin - Madison
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Mid-Term Project

Sanket Deshpande

Bose-Einstein Condensation of Ultra-Cold Atoms

Introduction

The phenomenon of Bose-Einstein Condensation, or BEC, was introduced almost 100 years ago by Albert Einstein in 1925, based on the work by Satyendra Nath Bose in 1924. BECs were experimentally demonstrated only 25 years back, in 1925 and led to the Nobel Prize in Physics in 2001 - shared by E.A. Cornell, Wolfgang Ketterle, and E. Wieman [1].

Today, there are several BEC experiments on earth, and beyond! There have been multiple successful sounding rocket-borne BEC experiments [2], and earlier this year, a BEC of Rubidium atoms was experimentally demonstrated onboard the International Space Station by the NASA Cold Atom Lab (CAL) [3]. BECs are also referred to as the "fifth state of matter", and have a wide range of applications spanning fundamental science to commercial technologies. A very interesting application is the ability to form an "atom laser" - which is analogous to a Laser, but is made up of matter waves, instead of light waves. This is possible because BECs allow us to form a coherent and collimated beam of atoms.

Figure 1: Astronaut Christina Koch installing the NASA CAL payload onboard the ISS. Source: NASA JPL

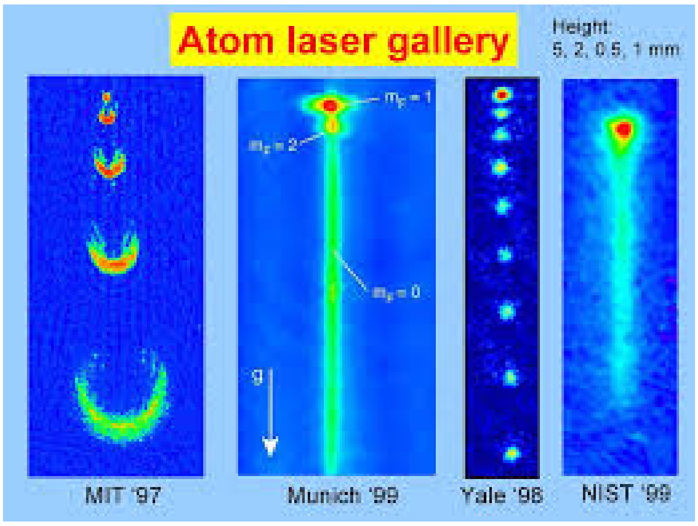

Figure 2: Atom laser from a BEC. Source: Ketterle Group, RLE, MIT

Bosons and Fermions

To understand BECs, we need to revise our understanding of elementary particles - which are generally divided into Bosons and Fermions. The primary criteria distinguishing them is their "spin". Particles exhibiting half-integer spins are categorised as Fermions while particles with integer spins are said to be Bosons. Hence, electrons, photons and neutrons are fermionic in nature, while photons, and the famed Higgs Boson are bosonic in nature. Another important feature is that fermions obey the Pauli Exclusion principle, while bosons do not. This implies that no two fermions can occupy the same state, but it is possible for multiple bosonic particles to be in the same state. This is illustrated further in figures 3 and 4.

Not just elementary particles, but atoms also exhibit bosonic or fermionic nature. If the atom exhibits a net integer spin, it exhibits bosonic nature and if it exhibits half-integer spin, then the atom exhibits fermionic nature. A simpler method to distinguish is based on the total number of fermions in the atom: for odd number of fermions, it exhibits fermionic nature; while for even number of fermions, it will exhibit bosonic nature. For example, Li-6 is said to be fermionic, while Li-7 is a bosonic atom. As we'll see later, this is an important property of bosons that leads to the formation of the condensate.

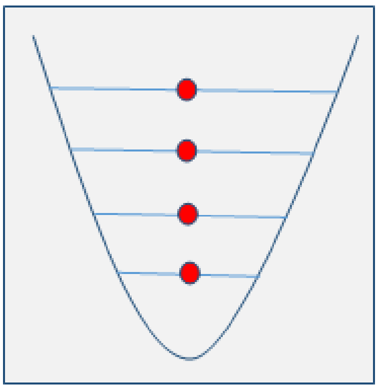

Figure 3: Fermions obey Pauli's Exclusion Principle

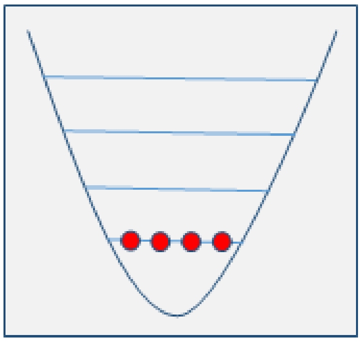

Figure 4: Bosons don't obey Pauli's Exclusion Principle

Quantum Statistics and Ultra-Cold Atoms

A bosonic gas follows Bose-Einstein statistics, and its statistical distribution is therefore denoted by the expression:

$$f_{BE}(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)} - 1} \tag{1}$$

Here, $\beta = 1/k_B T$ and μ is the chemical potential. Under this statistical distribution, multiple bosons can occupy the same energy state. More importantly, under the right conditions, all bosons in the ensemble avalanche to occupy the lowest energy state (or ground state), thereby leading to the formation of a condensate, or BEC. In contrast, fermions cannot cluster to the same state and hence densely occupy all possible, but distinct, energy levels. This is illustrated in Fig 5.

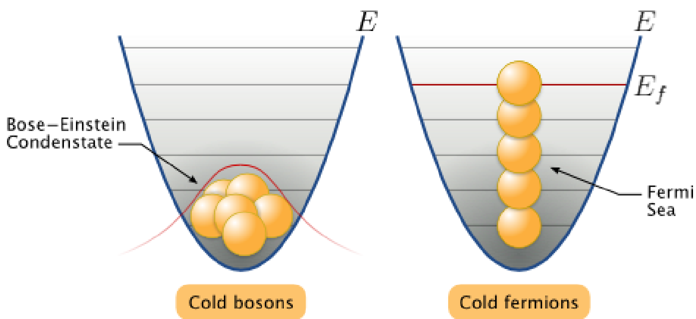

Figure 5: Bosons avalanche to the ground state. Fermions for a Fermi Sea

But, these effects aren't always significant - and hence aren't usually observed. For an ensemble of atoms at room temperature, there are several available energy levels, and the atoms conveniently occupy different energy levels - without competing with each other. The critical requirement for observing the "quantum" effects is to slow down the motion of the atoms, and hence obtain an ensemble of low-energy atoms. Since the Virial theorem relates the motion of atoms with their temperature, these slow atoms also exhibit low temperatures, and are hence known as "cold-atoms". In this "cold" regime, we're essentially forcing a lot of atoms to occupy energy levels under a certain threshold. Now, atoms start competing with each other to occupy these energy levels, and in the case of fermions, each one of them occupies one level. For bosons, they avalanche together to occupy the lowest-energy state.

How do we mathematically define the "cold" regime? Qualitatively, we need to make the atoms cool/slow enough such that their De-Broglie wavelength is of the same scale as the inter-atomic separation. Using quantum statistics, we determine that this condition is satisfied when the number density of the atoms satisfies the following condition:

$$n = \frac{2.6}{\lambda_{dB}^3} \tag{2}$$

The atoms are cooled by trapping them in a harmonic potential. In this potential well, we can relate their energy using the Virial theorem as:

$$\frac{1}{2}M\omega^2 r^2 \approx \frac{1}{2}k_B T \tag{3}$$

Hence, using equations 2 and 3, we can approximate the number of atoms trapped in the harmonic potential by the expression:

$$\mathcal{N}^{1/3} = \frac{k_B T_c}{\hbar\omega} \tag{4}$$

While we're forcing the atoms to reach the critical density (stated in equation 2), what prevents the atoms from condensing into a liquid instead? That's because the density is still very low; about 10^5 times lower than the density of air at ground level.

Inter-Atomic Interaction and GPE

At low temperatures, atoms are modelled as hard spheres, with radius of each atom equal to it's scattering radius [4], denoted here as a. In this cold ensemble, atoms interact with each other, which leads to an additional term in the Hamiltonian of every atom. For interaction between two atoms, this term is given as:

$$\frac{4\pi\hbar^2 a}{M}|\psi|^2$$

Hence, for interaction between $\mathcal{N}$ atoms, the term will be:

$$\frac{4\pi\hbar^2 a}{M}\mathcal{N}|\psi|^2$$

Therefore, writing the Schrodinger equation for an atom in this ensemble of trapped atoms:

$$\left\{-\frac{\hbar^2}{2M}\nabla + V(r) + \frac{4\pi\hbar^2 a}{M}\mathcal{N}|\psi|^2\right\}\psi = \mu\psi \tag{5}$$

This non-linear Schrodinger equation is known as the **Gross-Pitaevskii Equation**, or GPE. Usually, we define a quantity $g = \frac{4\pi\hbar^2 a\mathcal{N}}{M}$.

The solution to this equation can be modelled as a spherical gaussian, $\psi = Ae^{-r^2/2b^2}$, which exists between the radius $a < r < b$. Here, b is an arbitrary radial distance. The expression for energy can be obtained by substituting the wavefunction in the GPE.

$$E = \frac{3}{4}\hbar\omega\left\{\frac{a_{ho}^2}{b^2} + \frac{b^2}{a_{ho}^2}\right\} + \frac{g}{(2\pi)^{3/2}}\frac{1}{b^3} \tag{6}$$

To find the ground-state energy, we find the minima of the energy expression by differentiating it with respect to b. For $g = 0$, or the condition when the inter-atomic interaction term is very small, we obtain the ground state energy condition as, $b = a_{ho}$. And, a_{ho} is defined as the characteristic radius of this gaussian wavefunction,

$$a_{ho} = \sqrt{\frac{\hbar}{M\omega}} \tag{7}$$

Its interesting to observe that by substituting $b = a_{ho}$ and $g = 0$, we obtain the ground state energy as $E = \frac{3}{2}\hbar\omega$, which is the expected ground state energy of a quantum harmonic oscillator.

In a "cold" regime, the atoms are actually moving very slowly, and hence have minimal kinetic energy. This condition can be (approximately) mathematically illustrated as:

$$\mathcal{N} > \frac{a_{ho}}{a} \tag{8}$$

When this condition is satisfied, we can safely ignore the kinetic energy term in the GPE. This special condition is known as the **Thomas-Fermi regime**, and the Schrodinger equation can now be written as:

$$\{V(r) + g|\psi|^2\}\psi = \mu\psi \tag{9}$$

For a 3D Harmonic Potential:

$$V(x, y, z) = \frac{1}{2}M(\omega_x x^2 + \omega_y y^2 + \omega_z z^2) \tag{10}$$

We can determine the number density of the BEC trap to be:

$$n(x, y, z) = \frac{\mathcal{N}\mu}{g}\left(1 - \frac{x^2}{R_x^2} - \frac{y^2}{R_y^2} - \frac{z^2}{R_z^2}\right) \tag{11}$$

where $R_{x,y,z}$ are the edges of the trap, defined by:

$$\frac{1}{2}M\omega_{x,y,z}^2 R_{x,y,z}^2 = \mu \tag{12}$$

The chemical potential, μ, is determined by the normalisation condition

$$1 = \int\int\int |\psi|^2 dx\; dy\; dz \tag{13}$$

and is also denoted by the expression:

$$\mu = \hbar\bar{\omega} \times \frac{1}{2}\left(\frac{15\mathcal{N}a}{a_{ho}}\right)^{2/5} \tag{14}$$

where $\bar{\omega} = (\omega_x\omega_y\omega_z)^{1/3}$ is the mean oscillation frequency.

Cooling and Trapping Techniques

To successfully form a BEC, temperatures lower than 100 nK are expected, and cannot be reached using optical molasses and Doppler cooling techniques alone. We explore two important techniques that made formation of BECs possible:

Magnetic Trapping

The harmonic potential for trapping atoms is generated by establishing a radially-varying magnetic field, thereby taking advantage of the potential (energy) shifts experienced by atoms due to the Zeeman effect: $V = -\mu.\mathbf{B}$.
We create a magnetic field such that it varies linearly in the $x - y$ plane:
$\mathbf{B} = b'(x\hat{x}\ -\ y\hat{y})\ =\ b'r$
We also create a constant magnetic in the z-direction. So the the net magnetic field is given as: $\mathbf{B}\ =\ b'(x\hat{x}\ -\ y\hat{y})\ +\ B_o\hat{z}$
Therefore the magnitude of the field is:

$$|\mathbf{B}|\ =\ B_o^2 + (b'r)^{2\,1/2}\ \approx\ B_o + \frac{b'^2r^2}{2B_o}$$
$$\text{for}\ \ b'r << B_o$$

And the corresponding potential can be given as:

$$V(r) = g_F\mu_B M_F\left(B_o + \frac{b'^2r^2}{2B_o}\right) \tag{15}$$

$$V(r) = g_F\mu_B M_F B_o + \frac{1}{2}\frac{g_F\mu_B M_F b'^2}{B_o}r^2 \tag{16}$$

$$V(r) = V_o + \frac{1}{2}M\omega_r^2 r^2 \tag{17}$$

Hence, for the region near the center of the trap, we have established a harmonic potential, with angular oscillation frequency:

$$\omega_r = \sqrt{\frac{g_F\mu_B M_F}{MB_o}} \times b' \tag{18}$$

The V(r) vs r plot of this potential has a "round" bottom, as illustrated in Fig 6. This kind of trap is known as the "Ioffe Trap", and is constructed using current-carrying coils, as illustrated in Fig 7.

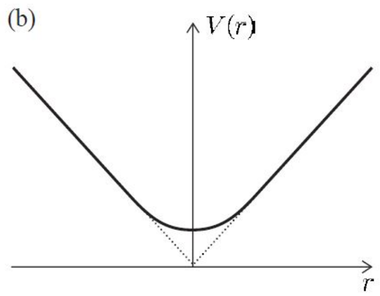

Figure 6: Harmonic Potential experienced by the atom near the center of the trap. [4]

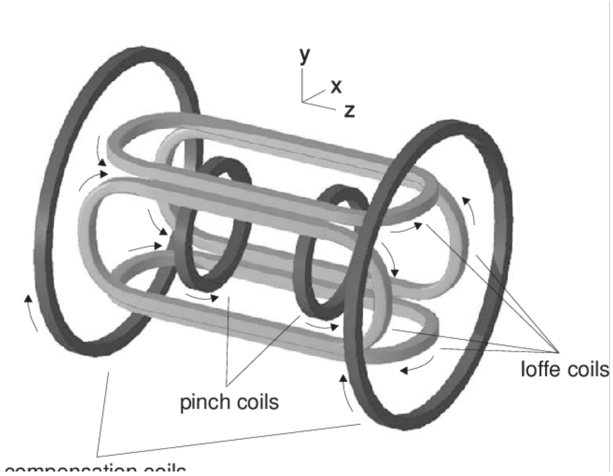

Figure 7: Illustration of the Ioffe Trap. [4]

Evaporative Cooling

A combination of laser and evaporative cooling is the key element for forming a BEC, hence, making it crucial for scientists to perfect the technique before attempting to form BECs. This led to a "race" between various research groups to perfect this technique. Fig 8 illustrates the reported results on evaporative cooling of alkali atoms, during the years leading up to the observation of the BEC.

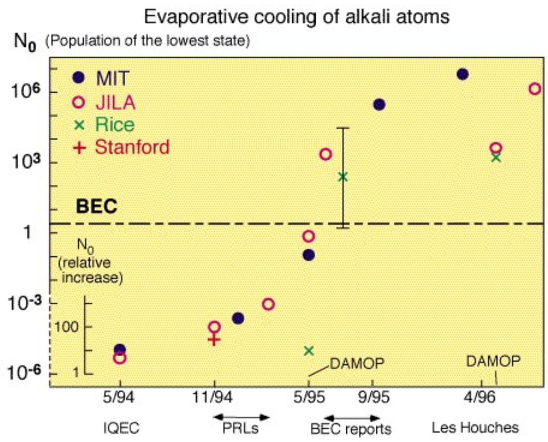

Figure 8: Illustrates the population achieved by various groups using evaporative cooling traps, leading up to the observation of the BEC.
Source: `https://www.rle.mit.edu/cua_pub/ketterle_group/intro/race/race.html`

This technique aims to make an ensemble of trapped atoms colder by removing those atoms that are "hotter" than a certain threshold temperature, thereby bringing down the overall temperature of the entire ensemble. If, at the start, the atoms have a Boltzmann distribution of energies as $\mathcal{N}(E) = \mathcal{N}_o \exp(-E/k_B T_1)$, with a characteristic temperature T_1. Now, all atoms with energies above a certain threshold, $E > E_{cut}$ are allowed to escape. Here, $E_{cut} = \eta k_B T_1$, and η is generally in the range 3-6. After the the atoms have established thermal equilibrium, the new distribution has lower temperature $T_2 < T_1$. This process is repeatedly to obtain the required ensemble of cold atoms. Fig 9 illustrates the concept further

During this process, the harmonic trap density increases: since the atoms get colder, they sink to a lower potential. This process can be attributed as *runaway evaporation*, which reduces the temperature of the entire ensemble by many orders of magnitude; thereby increasing the number density to the required value determined by Equation 2.

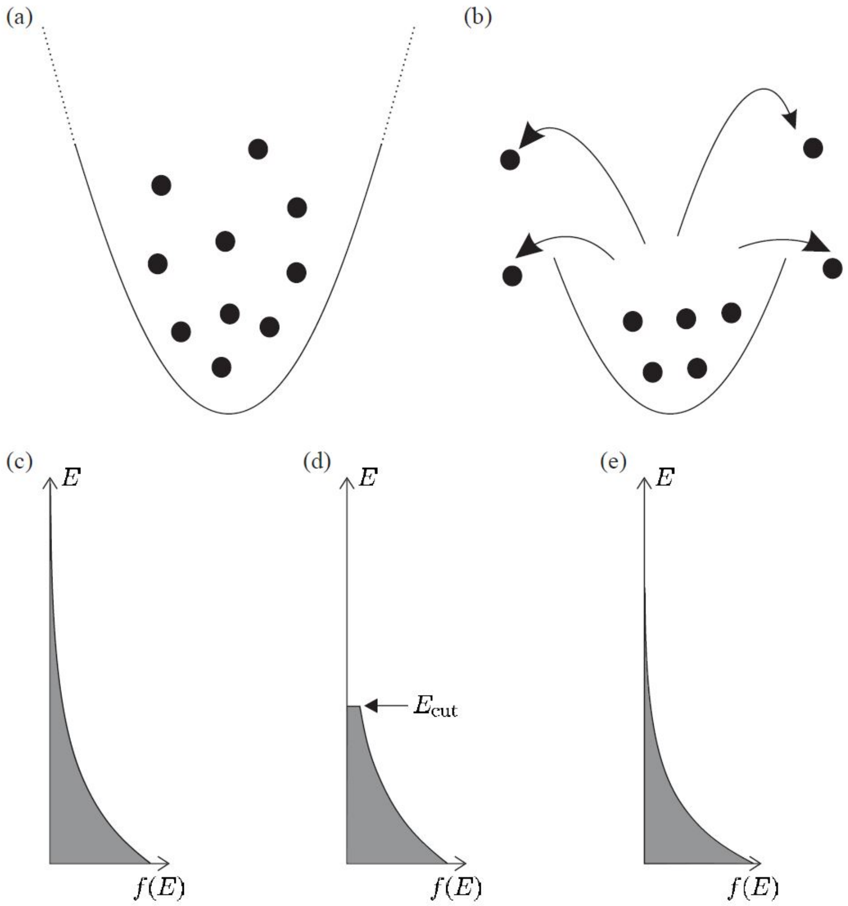

Figure 9: Illustration for evaporative cooling. The "hotter" atoms are allowed to escape from the trap, thereby reducing the overall temperature of all the remaining atoms in the trap. [4]

Numerical Modelling for a Na-11 atom BEC

I used `MATLAB` to build a numerical model of a BEC, for sodium atoms. Na-11 atoms are bosonic in nature, since they have even number of total fermions (11e + 11p +12n). The numerical model uses equations stated here in previous sections for determining some of the properties of the trap, and is used to obtain a plot of the expected number density in the $z = 0$ plane.

Inputs to the Numerical Model

The following quantities were used as input parameters to the numerical model. Source for this data is on Pg. 236, *Atomic Physics by Christopher J. Foot* [4].

Description	Symbol	Value
Scattering length (for Na)	a	2.9 nm
Radial Oscillation Freq (for x and y axes)	ω_x, ω_y	2π * 250 Hz
Axial Oscillation Freq (z axis)	ω_z	2π * 16 Hz
Harmonic Oscillator Length	a_{ho}	2 μm
Number of atoms in condensate	$\mathcal{N}$	10^6

Properties of the condensate

To form this condensate, a critical temperature of $T_c = 480.14\,nK$ is required, and therefore, the critical density required is $n_c = 2.06 \times 10^{13}\,cm^{-3}$.
For the stated values of the radial and axial harmonic oscillation frequencies, and for the required number of atoms to be trapped, we determine the chemical potential for the trap as, $mu/k_B = 130.4\,nK$. Hence, the BEC will confined to the following radial size of $R_x = R_y = 5.89\,\mu m$ and axial size of $R_z = 92.13\,\mu m$. The peak density at the center of the trap is $n_o = 18 \times 10^{13}\,cm^{-3}$
In the $Z = 0$ or, $X - Y$ plane, the number density forms an inverted parabola, indicating maximum density at the center of the trap. Fig 10 illustrates this conclusion further.

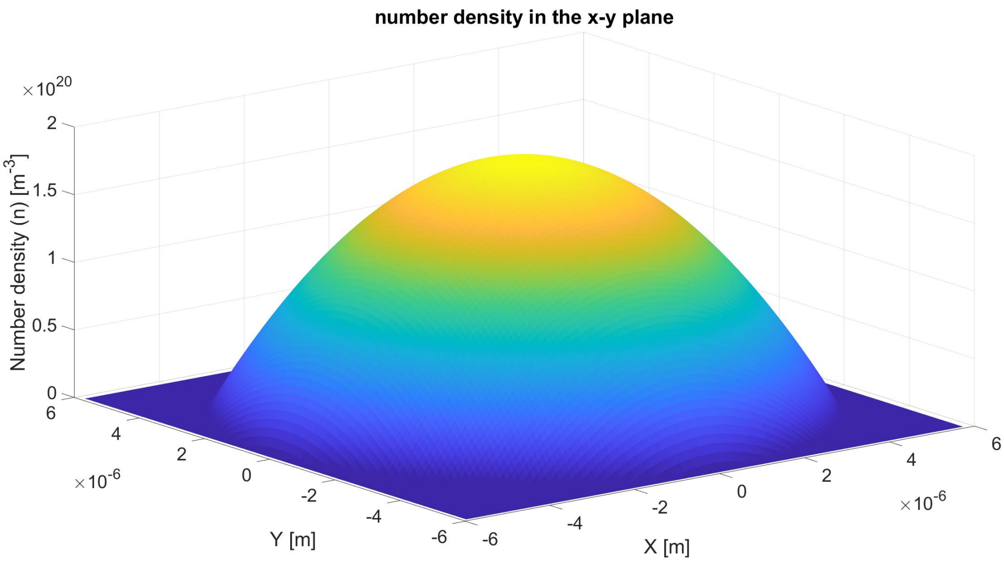

Figure 10: Inverted parabola shape of the number density, in the Z=0 plane.

MATLAB Script for the model

```
%EMA601 Mid-term project
%MATLAB scriptt to simulate sodium (Na-11) atom BECs
clear all

h=6.626e-34; %Planck's const in SI units
hb = h/(2*pi); %Reduced Planck's const in SI units
c=3e06; %speed of light in SI units
kb =  1.38e-23; %Boltzmann const in SI units

%defining initial parameters
a = 2.9e-9; %scattering length of sodium
wx = 2*pi * 250; %x-axis: angular oscillation freq
wy = wx; %y-axis: angular oscillation freq
wz = 2*pi * 16; %z-axis: angular oscillation freq
aho = 2e-6; %harmonic oscillator length
N = 1e06; %target number of atoms in the condensate


%determining secondary parameters
w = (wx*wy*wz)^(1/3) %average angular oscillation freq
M = hb/(w*aho^2); %mass of a sodium atom

%determining properties
Tc = hb*w*(N^(1/3))/kb %critical temperature for the trap
nc = 2.6/((h/sqrt(2*pi*M*kb*Tc))^3) %critical density of the trap
mu = hb*w*0.5*(15*N*a/aho)^(2/5) %chemical potential of the atoms
Rx = sqrt(2*mu/(M*(wx^2))) %x-axis: radial extent of the condensate
Ry = sqrt(2*mu/(M*(wy^2))); %y-axis: radial extent of the condensate
Rz = sqrt(2*mu/(M*(wz^2))) %z-axis: axial extent of the condensate
g = 4*pi*(hb^2)*N*a/M; %coupling const for inter-atomic interaction

%[X,Y,Z] = meshgrid(-100:1:100,-100:1:100,-100:1:100);
%X,Y,Z defined from -100 to 100 um, step size of 1 um

[X,Y] = meshgrid(-Rx:1e-7:Rx,-Ry:1e-7:Ry);
Z=0;
no = N*mu/g %number density at the center
n_range = no.*(1 - (X.^2)./(Rx^2) - (Y.^2)./(Ry^2) - (Z.^2)./(Rz^2));
n_range(n_range<0)=0;

clf(figure(1),'reset')
figure(1)
surf(X,Y,n_range, 'edgecolor', 'none')
title('number density in the x-y plane')
xlabel('X [m]')
ylabel('Y [m]')
```

```
zlabel('Number density (n) [m^{-3}]')
ax = gca;
ax.FontSize = 30;
%size(n_range);
```

References

[1] Wolfgang Ketterle. *Nobel lecture: When atoms behave as waves: Bose-Einstein condensation and the atom laser*. Reviews of Modern Physics, Vol 74, Oct 2002.

[2] Becker, D., Lachmann, M.D., Seidel, S.T. et al. *Space-borne Bose–Einstein condensation for precision interferometry.* Nature 562, 391–395 (2018).

[3] Aveline, D.C., Williams, J.R., Elliott, E.R. et al. *Observation of Bose–Einstein condensates in an Earth-orbiting research lab*. Nature 582, 193–197 (2020).

[4] Christopher J. Foot. *Atomic Physics.* `Ch10: Magnetic trapping, evaporative cooling and Bose-Einstein condensation.` Oxford University Press.