

## Lecture 2 BEC

Equipped with the Hartree approximation, which implies that the zero temperature multiparticle wave function may be well approximated by the product state with the common orbital satisfying the GP equation the question remains how good is this approximation. After all we know that the exact ground state must have a massively entangled form. If we knew this wave function then how we would determine “how many atoms are in the condensate and what is the condensate wave function?”. The formal answer to these questions was given more than 50 years ago by Onsager and Penrose. Here is what they propose:

Let  $\Psi(\vec{r}_1, \dots, \vec{r}_N)$  be the exact ground state. Since we consider bosons, this is a totally symmetric function of the arguments. Construct the one particle, reduced density matrix:

$$\rho(\vec{r}, \vec{r}') = \int \Psi(\vec{r}, \vec{r}_2, \dots, \vec{r}_N) \Psi^*(\vec{r}', \vec{r}_2, \dots, \vec{r}_N) d^3r_2 \dots d^3r_N \quad (1)$$

Of course this is a hermitian matrix of its position arguments. Hence we can write its spectral decomposition:

$$\rho(\vec{r}, \vec{r}') = \sum_j n_j \varphi_j^*(\vec{r}) \varphi_j(\vec{r}') \quad (2)$$

To secure a unit trace the eigenvalues must add-up to 1:

$$\sum_j n_j = 1 \quad (3)$$

The classics say: The presence of the condensate in the wave function (1) is manifested by the presence of a dominant single eigenvalue in the decomposition (2). The dominant eigenvalue is by definition a fraction of condensed atoms and its corresponding eigenfunction is the condensate wave function. This definition is easily tested on the case of the ideal gas. In this case the function (1) is just a product of the single particle ground states of the trap  $\varphi_0(\vec{r})$ . The reduction to one particle density matrix is trivial and for the ideal Bose gas we get:

$$\rho(\vec{r}, \vec{r}') = \varphi_0^*(\vec{r}) \varphi_0(\vec{r}') \quad (4)$$

with a single nonzero eigenvalue which is equal to 1 and an eigenfunction which is the ground state of the trap. Thus every atom is in the condensate, as it should be. Of course as we turn-on the interaction the dominant eigenvalue departs downward. The difference between 1 and the dominant eigenvalue is called the quantum depletion.

It is very hard to tell what is the value of the quantum depletion for actual dilute gas harmonic trap experiments but the estimate put this number at a few percent. On the other

hand an old example of the quantum degenerate Bose system,  $^4\text{He}$  is believed to have something close to 90% of atoms outside of the condensate.

A few years ago E. Lieb and coworkers have proved (under rather restrictive assumptions) that if the crucial interaction parameter  $f = an^{1/3}$  ( $n$  being a number density of atoms) tends to zero than the quantum depletion tends to zero and the only relevant eigenvector tends to the ground state of the GP equation.

Now, in a typical dilute gas experiment  $n \sim 10^{14} \frac{\text{atoms}}{\text{cm}^3}$ . Hence for instance for rubidium

$f \approx 1.24 \cdot 10^{-2}$ . We can use GP equation for this most standard condensate safely. One of the most beautiful aspect of quantum gases, however is the tunability of the scattering length with the help of a suitable magnetic field. The method is known as Feshbach resonance. You will hear about it this afternoon. This way one can make the interaction both: nearly vanishing and very strong departing from the realm of the GP equation, known in the trade as the mean field approximation.

Now let us look at the ground state of the GP equation. If we neglect the nonlinear collisions term, the ground state for the simplest case of the spherically symmetric harmonic trapping potential is just the standard Gaussian:

$$\psi(r) = N \exp\left[-\frac{m\omega}{2\hbar} r^2\right] \quad (5)$$

The width of the probability distribution is

$$d = \sqrt{\frac{\hbar}{m\omega}} \quad (6)$$

which is often used as a convenient unit of length. Such units are called “the oscillator units”.

As the number of atoms grows, the role of the nonlinear term grows as well. The interaction energy is proportional to the square of the number of atoms while the kinetic and the potential trap energy are linear functions of  $N$ . Let us assume for a moment the repulsive ( $a > 0$ ) interaction. The cloud must broaden with growing  $N$ . This way it also smoothes-out. The kinetic energy is proportional to the curvature of the wave function. As a result the relative role of the kinetic energy decreases. A drastic approximation, valid for standard condensate with more than 10000 atoms is to drop the laplacian altogether. This is called Thomas-Fermi approximation - a somewhat misleading name since the original TF approximation was for fermions - for multielectron atoms.

Once the laplacian is dropped we have just an algebraic equation:

$$\frac{1}{2}m\omega^2 r^2 \varphi + Ng |\varphi|^2 \varphi = \mu \varphi \quad (7)$$

Hence the nonzero solution is:

$$|\varphi|^2 = \frac{1}{Ng} \left( \mu - \frac{1}{2}m\omega^2 r^2 \right) \quad (8)$$

an inverted parabola which extends all the way until the density vanishes (it can not be negative!). The size of the parabola,

$$R_{\text{TF}} = \sqrt{\frac{2\mu}{m\omega^2}} \quad (9)$$

is called the Thomas-Fermi radius of the condensate. Of course for an asymmetric harmonic trap there are up to three different TF sizes. Now we have 2 unknowns:

$R_{\text{TF}}$  and  $\mu$ . We can compute both of them since we have an additional relation:

$$\int |\varphi|^2 d^3r = 1 \quad (10)$$

The integral is:

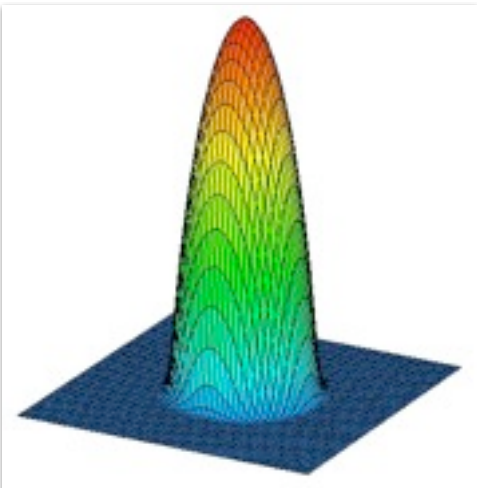
$$\frac{4\pi R^3}{Ng} \left( \frac{\mu}{3} - \frac{m\omega^2}{10} R^3 \right) = 1 \quad (11)$$

Substituting (9) into (11) we get:

$$R_{\text{TF}} = \left[ 15d^4 aN \right]^{1/5} \quad (12)$$

Note that  $N^{1/5}$  is a very weak dependence on the number of atoms and you should remember that in a typical experiment with 100000 to a few million atoms the Thomas Fermi radius is 5 to 6 times larger than the corresponding oscillator unit.

The TF solution is clearly wrong just at the edge. The GP equation has certainly differentiable solution. Thus it is no surprise that the exact solution has a gradual fall-off near the edge:



Just a quick look at the solution (8) indicates that something is deeply wrong if we try to apply it to the attractive gas. In fact attractive gas collapses if the number of atoms exceeds some threshold, typically rather small number. It is not hard to make a rough estimate of this threshold. Imagine bosons trapped in a spherical harmonic potential with the negative scattering length.

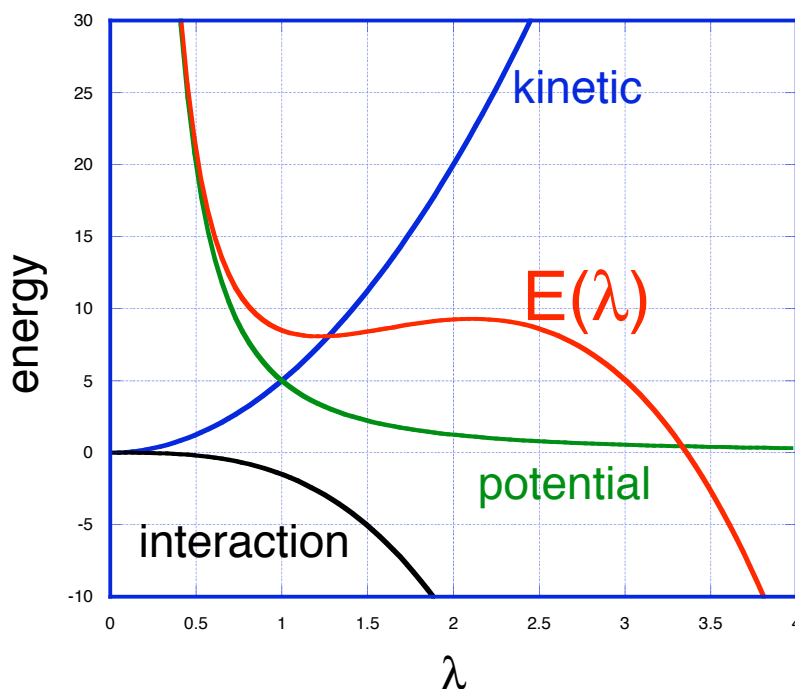
Suppose we write a trial wave function in a form discussed already in our BEC-1 lecture:

$$\psi_\lambda = \lambda^{3/2} \varphi(\lambda \vec{r}) \quad (13)$$

Functions in this family have all the same shape (we would typically chose Gaussian if interested in numerical values), are all normalized and differ by spatial scaling. We now take the energy functional and obtain, like in BEC-1:

$$E(\lambda) = \lambda^2 T + \lambda^{-2} V_{tr} + \lambda^3 E_{int} \quad (14)$$

The last term is now negative and proportional to the number of atoms.



We see a shallow minimum and it is clear that increasing the number of atoms we can make negative term win and the minimum will disappear. Thus there would be no stable solution of the GP equation. For the first condensate of lithium obtained by Randy Hulet at the beginning the situation was so confused that he was not among those considered for the Nobel prize. Now we know that in his trap he could hold a BEC containing about 2000 atoms.