Lecture 1 BEC

Till now only Bose-Einstein condensation of an ideal gas was discussed. Now we are going to make a great leap: we are going to include interactions. At the beginning we shall restrict our attention to the weakly interacting Bose gas at zero temperature. Thus, we want to study the ground state of the multiparticle hamiltonian:

$$H = \sum_{n=1}^{N} (\frac{p_n^2}{2m} + V_{tr}(\vec{r}_n)) + \frac{1}{2} \sum_{n \neq n'}^{N} V(\vec{r}_n - \vec{r}_{n'}) \qquad (1)$$

In most applications the trapping potential is just a more or less a symmetric harmonic oscillator potential. The inclusion of only binary interactions is well justified. The interatomic potential consists of a very short range repulsive part (present at distances of the order of atomic diameter) and of attractive tail coming from the interaction between induced electric dipoles. So, it falls-off rapidly ($\sim 1/r^6$ or if one includes the effects of retardation $\sim 1/r^7$).

Of course the ideal Bose gas consisting of *N* atoms at zero temperature has all atoms in the same single particle state, which is the ground state of the trapping potential. Thus the multiparticle wave function has a very simple product form:

$$\Psi(\vec{r}_1,..\vec{r}_N) = \prod_{n=1}^{N} \varphi(\vec{r}_n) \qquad (2)$$

This notion "each atom in the same state" should also apply to a condensate of weakly interacting atoms. Thus it makes sense to seek the approximate ground state of the hamiltonian (1) still in fully factorized form (2) optimizing the single particle orbital. We know the Ritz variational principle, so the optimal orbital should minimize the energy expectation value in the set of factorizable functions. It is a Hartree approach. (No need to invoke Fock - we deal with bosons, not with fermions).

We compute the energy functional of hamiltonian (1) in the product state (2):

$$E[\varphi] = N <\varphi | (T + V_{tr}) \varphi > + \frac{N(N-1)}{2} <\varphi\varphi | V\varphi\varphi > \qquad (3)$$

variation must be done with constraint fixing the normalization:

$$<\varphi | \varphi >= 1 \qquad (4)$$

Using the Lagrange multiplier in the form $N\mu$ we arrive at the functional:

$$F[\varphi] = E[\varphi] - N\mu <\varphi | \varphi > \qquad (5)$$

Postulating vanishing of the linear increment of this functional with respect to $\delta\varphi^*$:

$$\frac{\delta F[\varphi]}{\delta \varphi^*(\vec{r})} = 0 \qquad\qquad (6)$$

we get:

$$(\hat{T} + \hat{V}_{tr})\varphi(\vec{r}) + (N-1)\int \varphi^*(\vec{r}\,')V(\vec{r}\,'-\vec{r})\varphi(\vec{r}\,')d^3r\,'\,\varphi(\vec{r}) = \mu\varphi(\vec{r}) \qquad (7)$$

Our equation has a form of time independent, **nonlinear** Schrödinger equation with obvious interpretation of the last term as the action of N-1 atoms on the one for which the equation has been written.

There are 2 simplifications usually made at this point: First we shall omit 1 in comparison to N (~1000000). Second, in the dilute cold gas typical distances between atoms are huge compared to the range of the potential. Therefore one typically approximates the interatomic potential by Dirac delta function. Resulting equation is called the Gross-Pitaevski equation:

$$-\frac{\hbar^2}{2m}\Delta\varphi + V_{tr}\varphi + Ng\,|\,\varphi\,|^2\,\varphi = \mu\varphi \qquad\qquad (8)$$

Several remarks:

1. Condensed atoms are typically equipped with the magnetic moment. Dipole-dipole forces fall-off as $1/r^3$ so they have much longer range. In most cases they are tiny compared to the van der Waals forces, but sometimes (chromium!) become relevant. In this case delta function approximation is not valid.
2. There is an interesting subtlety with the delta function potential in 3D. See below.
3. Due to the nonlinearity, the total energy of the state obtained is **not** equal to $N\mu$:

$$E = N\mu - \frac{N^2}{2}g\int |\,\varphi\,|^4 d^3r \;. \qquad\qquad (10)$$

Now, back to the delta potential. As we remember from QM lectures, the scattering on the interatomic potential at very low velocity is reduced to the s-wave. The scattered part of the wave function in 3D is $\dfrac{e^{ikr}}{r}$ and cannot be multiplied by the delta function. In other words the standard s-wave solution of the free Schrödinger equation is not in the domain of the hamiltonian containing delta potential. Another way of seeing the difficulty is to solve first the scattering on a spherical step potential and then take the delta function limit. One can easily check that in this limit the scattering amplitude tends to zero. In several books the scattering amplitude on the delta potential is calculated approximately in the first Born approximation. Accidentally one gets correct result, but the procedure is flowed as the first Born approximation applies to **high** rater than **low** energy scattering.

In the 30-ties of the last century the problem with contact potential in 3D was solved by Breit and Fermi. They encountered this potential in connection with nuclear physics problems.

They proposed to use a minimal extension of a 3D delta (we are using the relative coordinate - we are in the center of mass frame of colliding identical particles):

$$V_r \varphi(r) = g\delta(\vec{r}) \frac{\partial}{\partial r}(r\varphi(r)) \tag{11}$$

Acting on function regular at the origin it is just a standard delta:

$$g\delta(\vec{r})(\varphi(r) + r\varphi'(r)) = g\delta(\vec{r})\varphi(0) \tag{12}$$

but for 1/r type functions it gives:

$$g\delta(\vec{r})\frac{\partial}{\partial r}(r\frac{\chi(r)}{r}) = g\delta(\vec{r})\chi'(0) \tag{13}$$

which is also an acceptable result. Much later, mathematicians proved that this is the only selfadjoint extension of the hamiltonian with zero range interaction in 3D.

All we need is to look at the s-wave radial equation. Its general form **outside** of the potential is

$$\psi(r) = \frac{\sin(kr + \delta_0)}{r} \tag{14}$$

where δ_0 is the s-wave scattering phase shift. The Schrödinger equation:

$$-\frac{\hbar^2}{2m}\Delta\psi + g\delta(\vec{r})(r\psi) = \frac{\hbar^2 k^2}{2m}\psi \tag{15}$$

in its singular part, due to a well known formula

$$\Delta\left(\frac{1}{r}\right) = -4\pi\delta(\vec{r}) \tag{16}$$

takes a form:

$$2\pi\frac{\hbar^2}{m}(\sin\delta_0)\delta(\vec{r}) + gk(\cos\delta_0)\delta(\vec{r}) = 0 \tag{17}$$

Thus, in the limit of $k \to 0$

$$\delta_0 \approx -\frac{gkm}{2\pi\hbar^2} \tag{18}$$

Remembering the definition of the s-wave scattering length a (see my QM10 lecture)

$$a = -\frac{\delta_0}{k} = \frac{gm}{2\pi\hbar^2} \tag{19}$$

We are ready now to express the coupling in the GP equation in terms of well defined physical parameter *a*. There is only one small point: As we remember, the equation for the relative coordinate contains **reduced** mass, thus we need additional factor of 2. Finally the coupling constant in the GP equation takes a form:

$$g = \frac{4\pi\hbar^2 a}{m} \tag{20}$$

Why we do not need to worry for the Fermi correction in the GP equation? Easy: It does not act on a function which is singular at $\vec{r} = \vec{r}\,'$.

Here are the typical values of the s-wave scattering length for the first three condensed species:

$$a = 5.77\,\text{nm} \quad \text{for} \quad {}^{87}\text{Rb}$$
$$a = 2.75\,\text{nm} \quad \text{for} \quad {}^{23}\text{Na} \tag{21}$$
$$a = -1.45\,\text{nm}\,\text{for} \quad {}^{7}\text{Li}$$

The sign of *a* is very important, as we shall see later. Although the full interatomic potential always has both an attractive and a repulsive part, since only the scattering length enters the GP equation, people often say that *a*>0 gas has repulsive and *a*<0 gas has an attractive interaction.

The GP equation and its time dependent extension is the most often solved equation in the cold atom physics.

Every solution of time independent GP equation must satisfy the virial condition. It is easily derived. In what follows we assume the harmonic binding, that is a trapping potential which is a quadratic function of the coordinate. Suppose a function $\varphi(\vec{r})$ is a normalized eigenstate of the GP hamiltonian. Consider a one parameter family of normalized trial functions:

$$\varphi_\lambda(\vec{r}) = \lambda^{3/2}\varphi(\lambda\vec{r}) \tag{22}$$

Let's compute the energy functional for (22):

$$E(\lambda) = \lambda^2 T + \lambda^{-2}V_{tr} + \lambda^3 E_{\text{int}} \tag{23}$$

The values of a mean kinetic, a mean potential and a mean interaction energy in the eigenstate $\varphi(\vec{r})$ are the coefficients. Now the function $E(\lambda)$ has a stationary point at $\lambda = 1$.

Hence:

$$2T - 2V_{tr} + 3E_{\text{int}} = 0 \tag{24}$$

which is the extension to GP equation of the well known relation for the harmonic oscillator: $T = V_{tr}$.