University of California, Berkeley
Physics 221b Spring 2004

Problem Set 6
due March 19, 2004

1. In class, we discussed the Hartree-Fock approximation for fermions, for instance for electrons in an atom. One can also consider the Hartree-Fock approximation for bosons, for instance atoms (such as Rubidium) in a Bose-Einstein condensate (BEC). We will consider a BEC in the case where these atoms are trapped, i.e. in some external potential restricting their movement (magnetically in this case). A common example is where each atom is in a harmonic oscillator potential, i.e. each atom has its own kinetic and potential term:

$$K.E. + V(r_i) = -\frac{\hbar^2\nabla_i^2}{2m} + \frac{m}{2}\omega^2 r_i^2 \tag{1}$$

All the atoms have the same mass m and trapping frequency ω but can have different positions r_i. The atoms interact with each other via an inter-atom potential with approximate cross section a^2. Essentially we take them to be hard spheres. However, as the form doesn't matter in detail here, we'll use

$$V(r'-r) = \frac{4\pi\hbar^2 a}{m}\delta(r'-r)\ . \tag{2}$$

The distance a is the effective scale where the potential deforms the wave functions and must be small enough relative to the density that the mean field approximation works well (i.e. the other wavefunctions aren't changed much by the particle of interest). In practice this is only a good potential to use perturbatively, rather than for exact wavefunction solutions, as these delta function potentials won't collide in three dimensions.

   (a) Consider the trial wavefunction

$$\Psi(x_1, x_2, ..., x_N) = \phi(x_1)\phi(x_2)\ldots\phi(x_N) \tag{3}$$

Consider the expectation value of the Hamiltonian in this state. Vary the expectation value of the Hamiltonian to find the Hartree equation for one atom in this system in the ground state, i.e. find H_H in

$$H_H(r_i, p_i)\phi(r_i) = \epsilon_0 \phi(r_i) \tag{4}$$

The factor ϵ_0 is the energy the system would lose if you took out one particle–thus it can be considered similar to a chemical potential. You do not need to write its explicit form here.

(b) Consider the wavefunctions $\phi(r)$ to vary slowly on the scale of the interaction (which is pointlike!), thus the kinetic energy is small compared to the other energies in the problem. (In practice, you want $Na > a_{ho} = \sqrt{\frac{\hbar}{m\omega}}$, the latter is the fluctuation scale in the external potential.) Also say that $N-1 \sim N$. With these approximations, rewrite equation 4 above to get a "Thomas-Fermi" (like) approximation for the density $N|\phi(r)|^2$ from the above equation, in terms of $\epsilon_0, \omega, r, a, m$ and sketch its shape as function of r. We take the density to be zero in the region where its definition goes negative. In this approximation you can also calculate $\epsilon_0 \sim \mu$ by requiring that $\int |\phi(r)|^2 d^3r = 1$.

(c) Compare the shape of $N|\phi(r)|^2$ above to the case where there is no inter-atom interaction and one just has a harmonic oscillator potential for each atom. If

$$\epsilon_0 = \frac{\hbar\omega}{2}\left(\frac{15Na}{a_{ho}}\right)^{2/5} \tag{5}$$

and $Na/a_{ho} \gg 1$, what does this say about the density at the origin in the two cases?

Note that in both of these cases there are spatial correlations in these condensates, not only momentum correlations.

2. Merzbacher *exercise* 22.13 . You can assume that we already know $\langle N_i \rangle$ from class or the book.

3. We derived the band-gap equation in class, showing that a bound state with zero momentum existed whose energy E_{bnd} solved $\Phi(E) = -\frac{1}{v_0}$

where

$$\begin{aligned}\Phi(E) &= \sum_k' \frac{1}{E-\epsilon_{k_1}-\epsilon_{k_2}} \\ &= \frac{V}{(2\pi)^3}\int_{k_f}^{k_a} d^3k \frac{1}{E-\epsilon_{k_1}-\epsilon_{k_2}}.\end{aligned} \tag{6}$$

The prime indicates that you consider states with $\epsilon_{k_f} \le \epsilon \le \epsilon_{k_a}$ in the sum, where ϵ_k is the fermi gas energy $k^2/2m$ of the electrons in the problem. This is shown explicitly in the second line.

(a) To see the role of the Fermi sea in the above, consider $\vec{k}_1 = -\vec{k}_2$ and $k_f = 0$, and find the condition for a bound state (i.e. a solution for $\Phi(E) = -1/v_0$ for $E < 0$) on v_0. This is not an involved calculation!

(b) If the pair of electrons has total momentum of magnitude K, rather than zero total momentum, what happens to the sum in the momentum above (top and bottom limits)? You can assume that the total momentum $K \ll k_f$ if you want to write down an expression. What does this do in turn to $\Phi(E)$ and thus the gap energy? You may want to use a picture to show what happens to the gap energy.

Please show your work so that the grader can give you credit for effort even if you get the wrong answer. Also, please try to make your work readable!