Physics 127c: Statistical Mechanics

Bose Condensation in Trapped Alkali Gases

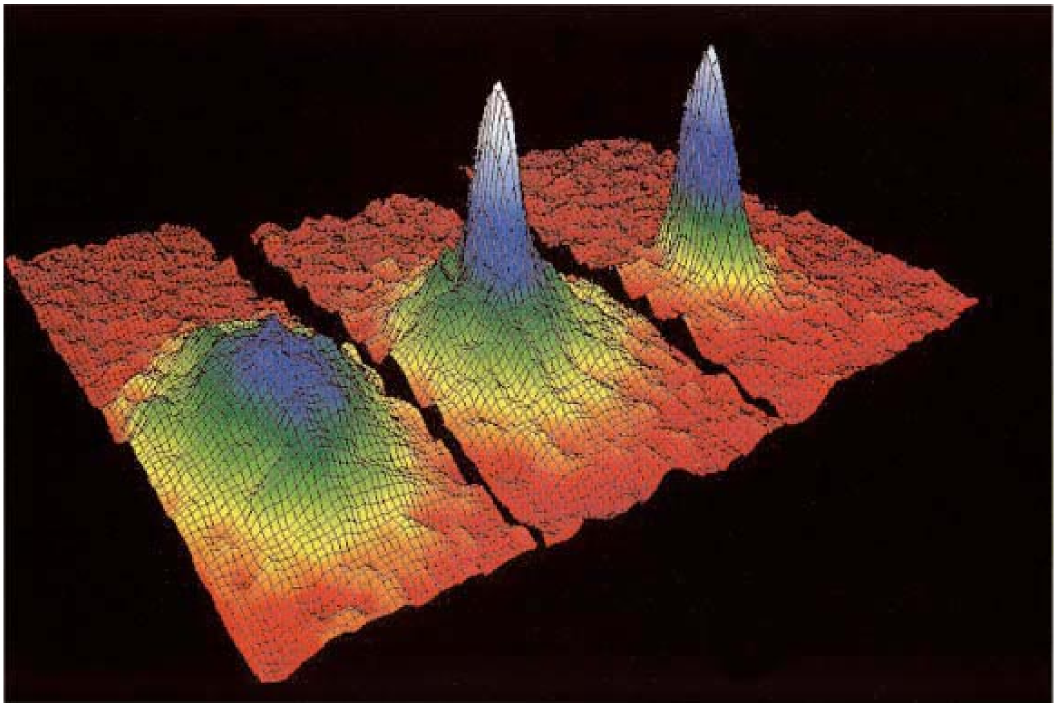

Figure 1: Observation of Bose-Einstein condensation of Rubidium atoms by Anderson et al. Science **269**, 198 (1995). The plots show the momentum distribution (measured by turning the trap off and letting the cloud freely expand) at successively lower temperatures.

In the past decade or so, Bose condensation has been produced in an entirely different parameter range than found in the only previously known laboratory system, liquid He^4. The system is alkali metal atoms trapped in magnetic or optical traps and cooled to very low temperatures. Parameters are $10^2 - 10^{10}$ atoms in traps of order tens of microns in extent, and cooled to 10^{-9} to 10^{-5}. Densities of $10^{11} - 10^{16}$ atoms/cm^3 are attained, compared with the 10^{21} atoms/cm^3 for He^4. Another difference is that the traps give a spatially varying environment, described by the trap potential $V_{ext}(\mathbf{r})$.

For a typical example, 10^6 atoms of Rb^{87} in a magnetic trap some parameters are: the Bose-Einstein condensation temperature $T_{BE} \sim 500$nK; the mean interaction energy $ng \sim 100$nK (n is the density and $g = \tilde{u}(0)$ the zero wave vector component of the pair interaction); and the zero point energy in the trapping potential $\frac{1}{2}\hbar\omega_0 \sim 5$nK (with ω_0 the oscillation frequency in the trapping potential). Interestingly, these numbers imply that interactions are relatively unimportant at T_{BE}, but are very important in the Bose condensed state. The particle separation is always large compared with the range of the pair potential, and a_s the "s-wave scattering length" that characterizes the scattering of a pair or particles. Because of this we can replace the atomic potential by an effective point scatterer

$$u(r) \simeq g\delta(r) = \frac{4\pi a_s \hbar^2}{m}\delta(r). \tag{1}$$

The phenomenon of Bose-Einstein condensation in these systems was first observed by meausring the collapse in of the position or momentum distribution. In a noninteracting picture, and approximating the trap potential as harmonic, the high temperature distribution is essentially classical ($k_B T \gg \hbar\omega_0$) so that

$$\left\langle x^2 \right\rangle_{CL} \sim k_B T / m\omega_0^2, \tag{2}$$

whereas Bose-Condensation into the ground state of the simple harmonic oscillator gives

$$\left\langle x^2 \right\rangle_{BE} \sim \hbar / m\omega_0. \tag{3}$$

Thus the collapse ratio would be estimated as

$$\sqrt{\frac{\left\langle x^2 \right\rangle_{CL}}{\left\langle x^2 \right\rangle_{BE}}} \sim \sqrt{\frac{k_B T_{BE}}{\hbar\omega_0}} \tag{4}$$

which is typically a factor of 10 or so. The ratio of the width of the momentum distributions is given by the same quantity. (Actually, as we will see, there are large corrections to these estimates from the interaction effects.) The first experiments measured this collapse, using free expansion to measure the momentum distribution, Fig. 1, or optical diffraction to measure the spatial extent [Andrews et al. Science **273**, 84 (1996)].

Bose-Einstein Condensation

We first generalize the notion of Bose-Einstein condensation to the spatially (and perhaps temporally) varying situation. Define the *one particle density matrix*

$$\rho(\mathbf{r}, \mathbf{r}', t) = \left\langle \psi^+(\mathbf{r}, t)\psi(\mathbf{r}, t) \right\rangle \tag{5}$$

with ψ the boson annihilation operator. In standard wavefunction notation this is

$$\rho(\mathbf{r}, \mathbf{r}', t) = N \sum_s p_s \int d^3r_2 \ldots d^3r_N \psi_N^{*(s)}(\mathbf{r}, \mathbf{r}_2, \ldots \mathbf{r}_N)\psi_N^{(s)}(\mathbf{r}', \mathbf{r}_2, \ldots \mathbf{r}_N) \tag{6}$$

which describes a statistical mixture of (symmetric) N particle states $\psi_N^{(s)}$. Considered as a matrix with respect to the coordinates $\mathbf{r}, \mathbf{r}'$ ρ is Hermitian, and so can be diagonalized in terms of some complete orthonormal set of one particle states χ_i

$$\rho(\mathbf{r}, \mathbf{r}', t) = \sum_i N_i(t)\chi_i^*(\mathbf{r}, t)\chi_i^*(\mathbf{r}', t) \tag{7}$$

with $N_i(t)$ the eigenvalues. Bose-Einstein condensation is said to occur if one or more of the N_i is $O(N)$. The condensation is "simple" if only one N_i is $O(N)$ (and then we label this one zero). The common situation where complex condensation occurs is when different spin components of the atoms are present. I will assume only one spin component is present, with fixed spin direction, and talk about them as spinless bosons, and only consider simple condensation. N_0 is then the condensate number. The order parameter can be conveniently defined as

$$\Psi(\mathbf{r}, t) = \sqrt{N_0(t)}\chi_0(\mathbf{r}, t). \tag{8}$$

Defining boson operators a_i, a_i^+ by

$$a_i(t) = \int d^3r \chi_i^*(\mathbf{r}, t)\psi(\mathbf{r}) \tag{9}$$

etc., then $\langle N_0 \rangle = \left\langle a_0^+ a_0 \right\rangle$. If we again use this to imply a_0 can be considered a classical number rather than an operator, and allow number-mixed states, we can describe the condensation as

$$\langle a_0 \rangle = N_0^{1/2}(t), \tag{10}$$

$$\langle \psi(\mathbf{r}, t \rangle = \Psi(\mathbf{r}, t). \tag{11}$$

Noninteracting Bosons

For noninteracting bosons we just need to study the statistical mechanics of condensation into the energy levels of the trap potential. This can usually be approximated as harmonic

$$V_{ext}(\mathbf{r}) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2), \tag{12}$$

with ω_i the oscillation frequencies along orthogonal axes. For simplicity I will usually assume the isotropic case, all $\omega_i = \omega_0$. Bose condensation in this potential is the subject of Homework 4.

Interaction Effects

If we imagine Bose condensation into the ground state of the harmonic potential for noninteracting particles, a very large density would be produced, so large for typical experimental parameters that the interactions would be very strong: we therefore must take the interactions into account in the Bose condensation.

An interesting observation is that to lowest order the interactions actually favor Bose condensation. Consider the average interaction energy for the point potential

$$\langle H_{int}\rangle = \frac{1}{2}g \int \left\langle \psi^+(\mathbf{r})\psi^+(\mathbf{r})\psi(\mathbf{r})\psi(\mathbf{r})\right\rangle d^3r. \tag{13}$$

Using the inverse of (9)

$$\psi(\mathbf{r}) = \sum_i \chi_i(\mathbf{r})a_i \tag{14}$$

this can be written

$$\langle H_{int}\rangle = \frac{1}{2}g \sum_{ijkl} \left\langle a_i^+ a_j^+ a_k a_l\right\rangle \int \chi_i^*(\mathbf{r})\chi_j^*(\mathbf{r})\chi_k(\mathbf{r})\chi_l(\mathbf{r}) d^3r. \tag{15}$$

If we calculate the average of the product of four operators in Hartree-Foch spirit keeping all nonzero pair averages

$$\left\langle a_i^+ a_j^+ a_k a_l\right\rangle \simeq \left\langle a_i^+ a_k\right\rangle \left\langle a_j^+ a_l\right\rangle + \cdots \tag{16}$$

$$= N_i \delta_{ik} N_j \delta_{jl} + \cdots \tag{17}$$

then we find

$$\langle H_{int}\rangle = \frac{1}{2}g \sum_{ij} N_i N_j (2-\delta_{ij}) \int |\chi_i(\mathbf{r})|^2 \left|\chi_j(\mathbf{r})\right|^2 d^3r, \tag{18}$$

since for the $i = j$ term there is only one choice of operators, whereas for $i \neq j$ the pairings can be chosen in two ways. Because of the factor $2 - \delta_{ij}$ the interaction energy is twice as large for the “split” condensation $N_1 = N/2$, $N_2 = N/2$ as for $N_1 = N$, assuming the integral factor is about the same. This would not be true for distinguishable particles. Thus the interaction and statistics further favor occupation of a single state.

Gross-Pitaevskii Equation

Using the simplicity of the weak, point interactions allows the derivation of a differential equation for the order parameter. I will confine myself to zero temperature, so to lowest order in the interactions all the particles are condensed $N_0 = N$ and

$$\psi_N(\mathbf{r}_1, \ldots \mathbf{r}_N) = \prod_{i=1}^{N} \chi_0(\mathbf{r}_i), \tag{19}$$

with χ_0 to be determined. The self-consistent best single-particle state for condensation is given by minimizing the total energy

$$\langle H\rangle_N \simeq N\int d^3r\left\{\frac{\hbar^2}{2m}\left|\nabla\chi_0(\mathbf{r})\right|^2+V_{ext}(\mathbf{r})\left|\chi_0(\mathbf{r})\right|^2\right\}+\frac{1}{2}N^2g\int d^3r\left|\chi_0(\mathbf{r})\right|^4. \tag{20}$$

(Actually evaluating the integral or calculating $\left\langle a_0^+a_0^+a_0a_0\right\rangle_N$ gives a factor of $N(N-1)$ rather than N^2 in the last term. However for large N we can ignore the difference.) Minimizing with respect to χ_0 maintaining the normalization $\int|\chi_0|^2=1$ gives

$$-\frac{\hbar^2}{2m}\nabla^2\chi_0+V_{ext}\chi_0+Ng\left|\chi_0\right|^2\chi_0=\mu\chi_0, \tag{21}$$

where μ arises as the Lagrange multiplier of the normalization constraint. Multiplying by χ_0^* and integrating gives

$$\mu=\int d^3r\left\{\frac{\hbar^2}{2m}\left|\nabla\chi_0(\mathbf{r})\right|^2+V_{ext}(\mathbf{r})\left|\chi_0(\mathbf{r})\right|^2\right\}+Ng\int d^3r\left|\chi_0(\mathbf{r})\right|^4=\frac{\delta\langle H\rangle_N}{\delta N} \tag{22}$$

(where in the last result $\delta\langle H\rangle_N/\delta\chi_0=0$ has been used). Thus μ is indeed the chemical potential. Writing $\Psi=N^{1/2}\chi_0$ then gives the conventional form of the Gross-Pitaevskii equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r})+V_{ext}(\mathbf{r})\Psi(\mathbf{r})+g\left|\Psi(\mathbf{r})\right|^2\Psi(\mathbf{r})=\mu\Psi(\mathbf{r}). \tag{23}$$

Since χ_0 is normalized to unity $\int|\Psi|^2d^3r=N$.

Equation (23) can also be derived from the stationarity condition for the boson operator

$$[\psi(\mathbf{r}),H]=0, \tag{24}$$

and then replacing $\psi\to\langle\psi\rangle=\Psi$ everywhere.

An important property of the condensed trapped gases is uncovered by considering the solution in a box of size L^3 with impenetrable walls. Near one wall (say at $x=0$) the behavior is given by the 1d GP equation with $V_{ext}=0$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x)+g\Psi^3(x)=\mu\Psi(x) \tag{25}$$

with boundary condition $\Psi(0)=0$. You can check that the solution to the equation is

$$\Psi(x)=n^{1/2}\tanh(z/\sqrt{2}\xi) \tag{26}$$

with n the density in the bulk far from walls and $\mu=ng$. The *healing length* ξ is given by

$$\xi=\sqrt{\frac{2mng}{\hbar^2}}=(8\pi na_s)^{-1/2}. \tag{27}$$

The length ξ is the distance over which variations of the magnitude of the order parameter tend to occur. It satisfies

$$\frac{\xi}{a_s}=(8\pi na_s^3)^{-1/2}\gg 1. \tag{28}$$

Thomas-Fermi Approximation

We now return to the case of trapping in the harmonic potential V_{ext}. Usually in atomic traps $\xi \ll a_{ho}$ with $a_{ho} = (\hbar/m\omega_0)^{1/2}$ the width of the ground state wave function in the harmonic well. This means that the gradient term in the GP equation can be ignored, except near the surface of the gas where $\Psi \to 0$. This gives a local or *Thomas-Fermi* approximation

$$|\Psi(\mathbf{r})|^2 = \frac{\mu - V_{ext}(\mathbf{r})}{g}, \tag{29}$$

so that the density of condensate is just such that the chemical potential is constant after taking into account the repulsive interaction, i.e. the potential well is "filled up" to the chemical potential.

For an isotropic harmonic potential

$$|\Psi(\mathbf{r})|^2 = \frac{\mu - \frac{1}{2}m\omega_0^2 r^2}{g} \tag{30}$$

the total number of particles is given by integrating out to the radius R where $\frac{1}{2}m\omega_0^2 R^2 = \mu$. This gives

$$R = \left(\frac{15}{4\pi}\frac{Ng}{m\omega_0^2}\right)^{1/5} = (15Na_s a_{ho}^4)^{1/5}. \tag{31}$$

Hence

$$\frac{R}{a_{ho}} = \left(15N\frac{a_s}{a_{ho}}\right)^{1/5}. \tag{32}$$

This number is typically of order 5 to 10 for the trapped gases, so that the width of the condensed ball of gas is significantly wider than given by the noninteracting theory. This ratio determines the relative importance of interaction and trap-potential effects.

Time Dependent Gross Pitaevskii Equation

Generalizing Eq. (24) to the time dependent equation, and following the same procedure gives the time dependent Gross-Pitaevskii equation

$$i\hbar\frac{\partial\Psi(\mathbf{r},\mathbf{t})}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},\mathbf{t}) + V_{ext}(\mathbf{r})\Psi(\mathbf{r},\mathbf{t}) + g\,|\Psi(\mathbf{r},\mathbf{t})|^2\,\Psi(\mathbf{r},\mathbf{t}). \tag{33}$$

The stationary solution is given by setting $\Psi(\mathbf{r},\mathbf{t}) = e^{-i\mu t/\hbar}\Psi(\mathbf{r})$, incidentally verifying the Josephson evolution equation for the phase of the order parameter.

Excitations

We can look for the solution of excitations oscillating at some frequency ω

$$\Psi(\mathbf{r},t) = \Psi_0(\mathbf{r})e^{-i\mu t/\hbar} + \delta\Psi(\mathbf{r},t) \tag{34}$$

with $\delta\Psi$ small and $|\Psi_0(\mathbf{r})|^2$ related to μ and $V_{ext}(\mathbf{r})$ as before. Substituting into Eq. (33) and linearizing in $\delta\Psi$ gives

$$i\hbar\frac{\partial\delta\Psi(\mathbf{r},\mathbf{t})}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\delta\Psi(\mathbf{r},\mathbf{t}) + V_{ext}(\mathbf{r})\delta\Psi(\mathbf{r},\mathbf{t}) + g\,|\Psi_0(\mathbf{r},\mathbf{t})|^2\,\delta\Psi(\mathbf{r},\mathbf{t}) + g\Psi_0^2(\mathbf{r},\mathbf{t})\delta\Psi^*(\mathbf{r},\mathbf{t}). \tag{35}$$

The involvement of both $\delta\Psi$ and $\delta\Psi^*$ in this equation suggests the trial solution

$$\delta\Psi(\mathbf{r},t) = e^{-i\mu t/\hbar}\left[u(\mathbf{r})e^{-i\omega t} + v^*(\mathbf{r})e^{i\omega t}\right]. \tag{36}$$

Substituting and picking out the pieces varying as $e^{\pm i\omega t}$ gives

$$\hbar\omega u(\mathbf{r}) = [H_0 - \mu - 2g\,|\Psi_0(\mathbf{r})|^2]u + g\Psi_0^2(\mathbf{r})v \tag{37}$$

$$-\hbar\omega v(\mathbf{r}) = [H_0 - \mu - 2g\,|\Psi_0(\mathbf{r})|^2]v - g\Psi_0^{*2}(\mathbf{r})u \tag{38}$$

with $H_0 = -(\hbar^2/2m)\nabla^2 + V_{ext}$. These are a special case ($\partial/\partial t \to \pm i\omega$) of the *Bogoliubov-deGennes* equations. For the free space case $V_{ext} = 0$, $\Psi_0(\mathbf{r}) = n^{1/2}$, $\mu = ng$, and $u(\mathbf{r}), v(\mathbf{r}) \propto e^{i\mathbf{q}\cdot\mathbf{r}}$. This gives

$$\omega = \sqrt{\left(\frac{\hbar^2 q^2}{2m}\right)^2 + \hbar^2 q^2\left(\frac{ng}{m}\right)}. \tag{39}$$

This is exactly the Bogoliubov spectrum.

Collective Mode, Hydrodynamics

In the limit where the interactions dominate the Gross-Pitaevskii or Bogoliubov-deGennes equations reduce to familiar hydrodynamic equations for the superfluid velocity coupled to the density. Introducing magnitude and phase variables for the order parameter

$$\Psi(\mathbf{r},t) = \sqrt{n(\mathbf{r},t)}e^{i\Phi(\mathbf{r},t)} \tag{40}$$

the time dependent GP equation can be expressed as

$$\frac{\partial n}{\partial t} + \nabla\cdot(\mathbf{v}_s n) = 0, \tag{41a}$$

$$m\frac{\partial \mathbf{v}_s}{\partial t} + \nabla\cdot\left(V_{ext} + ng + \frac{1}{2}mv^2 - \frac{\hbar^2}{2m\sqrt{n}}\nabla^2\sqrt{n}\right) = 0, \tag{41b}$$

with $\mathbf{v}_s = (\hbar/m)\nabla\Phi$ as usual. The last term in the second equation, known as the quantum pressure, is often small (e.g. at long enough wavelengths). The equations then take the usual form of hydrodynamic equations for the broken symmetry variable Φ and the conjugate variable n.

An important application of the use of Eqs. (41) is in the collective modes of the trapped condensate in the trap potential. For example for the harmonic trap Eq. (12). The steady state solution has the density variation n_0 given by

$$V_{ext}(\mathbf{r}) + gn_0(\mathbf{r}) = \mu. \tag{42}$$

Small oscillations about this solution follow the equations ($\mathbf{v}_s$, δn small, neglect the quantum pressure term)

$$\frac{\partial \delta n}{\partial t} + \nabla\cdot(\mathbf{v}_s n_0(\mathbf{r})) = 0, \tag{43}$$

$$m\frac{\partial \mathbf{v}_s}{\partial t} + \nabla\cdot(g\delta n) = 0. \tag{44}$$

Together with Eq. (42) these give

$$m\frac{\partial^2\delta n}{\partial t^2} = \nabla\cdot\left[c^2(\mathbf{r})\nabla\delta n\right], \tag{45}$$

where $c(\mathbf{r}) = \sqrt{(\mu - V_{ext}(\mathbf{r}))/m}$ plays the role of a position dependent speed of sound.

These equations are useful for understanding the oscillations of the trapped condensate in experiment, e.g. Fig. 2.

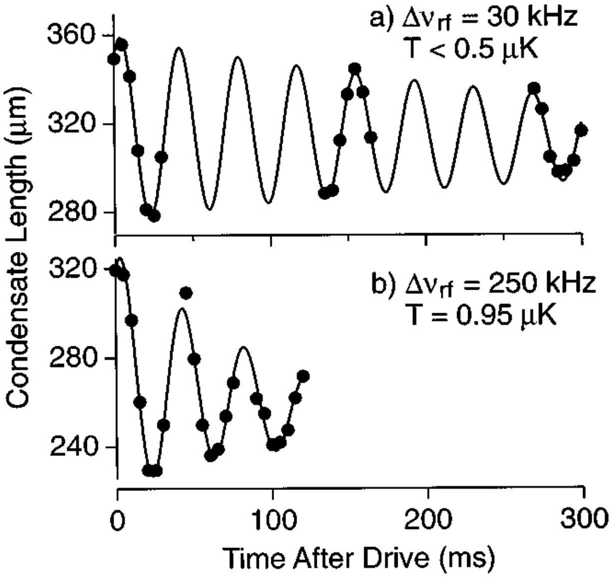

Figure 2: Oscillations in the axial width of the trapped gas ($m = 0$ mode) at low and high temperatures. [From Stamper-Kurn et al., Phys. Rev. Lett.**81**, 500 (1998)]

Other Applications

The Gross-Pitaevski equation provides a simple approach to study other interesting questions, such as vortex lines in rotating samples, the Josephson effect, and the phase interference of two condensed clouds (for the latter see the paper by Röhrl et al., Phys. Rev. Lett. **78**, 4143 (1997)).

Further Reading

Leggett (the 2003 Nobel Prize winner) has a nice review article on the basic physics of Bose-Eisntein condensation in the context of atomic traps, Rev. Mod. Phys. **73**, 307 (2001). Sections IID, IIE, III, IVD, and V are particularly relevant. The other sections go into topics I have not covered, such as the multiplicity of hyperfine levels, a careful discussion of the pair interaction, Bogoliubov theory, and the Josephson effect. An idiosyncrasy of Leggett (which may be correct!) is that he does not like the approach that has become common (and which I have used) of assuming a nonzero value for the expectation value of a creation or annihilation operator, which requires number-mixed states: he tries to avoid this approach wherever possible. An early reference on the application of the Gross-Pitaevskii equation is *Baym and Pethick*, Phys. Rev. Lett. **76**, 6 (1996). You could also look at one or more of the Nobel lectures referenced in the context of Homework 7 in Ph127a.

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