Quantum dynamics of atomic matter waves

We now turn to the quantum properties of matter fields.  
• As the atomic temperature approaches zero, the quantum statistics of the atoms become increasingly important. As an ensemble of non-interacting, bosons is cooled $T \rightarrow 0$, a macroscopic number of atoms occupy the ground state.  
• Advances in laser cooling and trapping techniques have allowed experiments to probe this quantum degenerate state of an atomic gas. In the case of bosonic atoms, the most prominent example of such a state is a Bose-Einstein condensate (BEC).

Introduction:  
• A gas at high temperature should behave classically, with each atom behaving like a point particle with a well-defined position and momentum.  
• At low temperature, the atoms are best described as matter wave packets, whose size is set by the deBroglie wavelength

$$\lambda_{dB} = \sqrt{\frac{2\pi \hbar^2}{mk_BT}}.$$  

• When the atomic wave-packets start to overlap in position, the quantum statistics of the atoms becomes important.  
• The transition between primarily classical and primarily quantum mechanical behavior occurs when the density $n$ and the temperature $T_c$ satisfy

$$n \lambda_{dB}(T_c)^3 = |$$

$$k_BTc = \frac{2\pi \hbar^2}{m\lambda_{dB}^2} = \frac{2\pi \hbar^2}{m} n^{2/3}.$$  

For Bose atoms below this critical temperature, $0 < T < T_c$, a macroscopic
number of atoms will occupy the lowest energy state—even at finite temperature. This so-called Bose condensation will occur only if the atom cloud is both dense and cold, which means that the phase space density must be large.

\[ n \lambda_{dB}(T)^3 > 1 \]
Bose-Einstein statistics

- Bose-Einstein statistics describe the behavior of indistinguishable particles with integer spin, and thus determine how an ensemble of N identical Bose atoms with some total energy E will distribute themselves among the possible energy states.

- Distinguishability plays in determining this distribution. From statistical mechanics, we know that the weight of a certain arrangement of atoms is given by the number of ways that arrangement can be formed – or, in some sense, how random that arrangement is. The distinguishability of particles plays a crucial role in determining this weight.

- For example, consider 10 particles distributing themselves between two states.

  Distinguishable, the statistical weight of the {5, 5} arrangement is 252 times
  Indistinguishable, the statistical weight of the {5, 5} arrangement is 1.

- In the grand canonical ensemble, N Bose particles with total energy E will distribute themselves among a set of energy levels according to the Bose-Einstein distribution,

\[ n_i = \frac{1}{e^{(\epsilon_i - \mu)/k_B T} - 1}, \]

\[ N = \sum_i n_i \]

\[ E = \sum_i \epsilon_i n_i. \]

where \( n_i \) is the number of particles occupying energy level \( \epsilon_i \).
At sufficiently low temperature, the most random distribution is obtained by putting a large fraction of the atoms into the ground state $\epsilon_0$ and letting the remaining atoms occupy higher energy states.

Since the number of atoms populating state can not exceed

$$\frac{1}{\left(\frac{\epsilon_i - \epsilon_0}{\hbar \omega}\right) - 1} \quad (\mu \leq \epsilon_0)$$

It the total # of particles in excited states is less than $N$, the remainder particles must be accommodated in the lowest single particle state whose population can be arbitrary large.

For $T < T_c$, for a non-interacting gas the number of atoms in excited states is

$$N_{ex} = \int \frac{D(\epsilon) \, d\epsilon}{\exp \left( \frac{\epsilon}{\hbar \omega T} \right) - 1} \quad \epsilon_0 = \beta = \mu$$

$$N_{ex} \sim N \left( \frac{T}{T_c} \right)^{3/2} \quad \text{ideal and unconfined}$$

where $D(\epsilon)$ is the density of states appropriate to the geometry of the problem.

- For non-interacting and unconfined bosons, the macroscopic ground state occupation number is

$$N_{g.s.} = N \left( 1 - \left( \frac{T}{T_c} \right)^{3/2} \right).$$

where $N$ is the total number of atoms and $T_c$ is the condensation temperature.

- When the atoms are confined to a three-dimensional harmonic oscillator trap:
\[ N_{g.s.} = N \left( 1 - \left( \frac{T}{T_c} \right)^3 \right). \]

In reality, however, even the dilute atomic gases interact, and even weak interactions can have a large effect on the dynamics of the condensate

**Experimental History**

- Superfluid helium was discovered and explored many decades before the recent advent of Bose condensation in atomic gases, and in some sense represents the first experimental evidence for BEC.
- However, liquid helium is a strongly correlated fluid, and bears little resemblance to the non-interacting ideal gas for which Bose condensation was first envisioned. Only about 10% of the helium atoms are in the ground state in superfluid helium; the rest compose coherent excitations which nevertheless exhibit superfluid behavior.
- One can thus consider superfluid helium to be a Bose condensate with a strong quantum depletion imposed by the strong interactions between atoms.
- For many years it was believed that Bose condensation in a gas was impossible. The constraints of temperature and density required to reach the critical temperature for condensation cannot be attained for gaseous material in thermodynamic equilibrium, because all materials become solid or liquid long before they are cold and dense enough to Bose condense.

- While there is no stable regime for BEC in a gas, one might hope to use a metastable state to realize condensation which would last long enough to measure.
- Spin-polarized hydrogen was the first candidate proposed, because the metastable triplet state of hydrogen has no bound state. Spin-polarized hydrogen therefore cannot recombine into H\(_2\), and left undisturbed remains polarized for days. Early contributors to this field included Isaac Silvera, Walraven, Dave Pritchard, and Dan Kleppner.
- However, at low temperatures, the hydrogen BEC experiments ran into a problem: whereas collisions with the walls typically did not flip the H spin at high temperatures, at low temperatures the density of H on the walls was high enough that spin-flip collisions became inevitable.
- Following the advent of laser cooling, many of the techniques pioneered by proponents of hydrogen BEC were adopted and
adapted for use with the alkali atoms.

- Those atoms, however could be cooled and trapped using a magneto-optical trap and optical molasses before transfer to a magnetic or off-resonant optical trap for evaporative cooling.
- This evaporative cooling step could only succeed for atoms whose elastic scattering rate far exceeds their inelastic scattering rate.
- By working at very low densities – and pursuing very low temperatures in the nano-Kelvin regime – researchers were able to find a stability window for the alkali gases, where recombination into bound states was extremely unlikely. In this regime, recombination requires a three-particle collision to satisfy energy and momentum conservation.
- For very low densities the three-body recombination rate is small compared to the two-body elastic scattering rate, allowing effective evaporative cooling.

Evaporative cooling

Once atoms are confined within a trap, further cooling techniques can be applied to them. Evaporative cooling has provided the most effective method for reaching ultracold temperatures, and the only technique for creating quantum degenerate gases. The physical mechanism behind evaporative cooling is very simple:

a. Those atoms which "boil off" the top of the trap must have more energy than the atoms remaining behind.

b. Once the remaining atoms re-thermalize, their temperature should go down
Quantum theory of an interacting Bose gas

A weakly interacting, dilute atomic gas can be well described by a Hamiltonian which incorporates single-particle terms and two-body interactions,

\[ \hat{H} = \sum_{i=1}^{N} \left( \frac{p_i^2}{2m} + V_{\text{trap}}(r_i) \right) + \sum_{\langle ij \rangle} V_{\text{int}}(r_i - r_j), \]

In cold, dilute atomic gases, the interaction potential can be replaced by the s-wave pseudo-potential

\[ V_{\text{int}}(r) \approx \frac{4\pi\hbar^2a}{m} \delta(r), \]

Second quantization

The second quantization formalism for matter waves resembles closely the methods used to quantize the electromagnetic field. As for photons, we will consider a complete set of single-atom states \{\ket{\zeta_i}\}, and define creation and annihilation operators which can add or remove an atom from those states

\[ \hat{b}_\zeta \ket{\text{vac}} = \ket{\text{vac}} \]
\[ \hat{b}_\zeta^\dagger \ket{\text{vac}} = \ket{\zeta}. \]
The statistics of the atoms determine the commutation properties of these operators.

\[
\begin{align*}
\text{Bosons:} & \quad [\hat{b}_\zeta, \hat{b}^\dagger_{\zeta'}] = \delta_{\zeta, \zeta'} \\
\text{Fermions:} & \quad \{\hat{b}_\zeta, \hat{b}^\dagger_{\zeta'}\} = \delta_{\zeta, \zeta'}.
\end{align*}
\]

where \([A,B] = AB - BA\) is the commutator and \([A,B] = AB + BA\) is the anticommutator. Since the commutation relations guarantee the symmetry or anti-symmetry of the resulting wave-functions, this formalism provides a convenient tool for treating indistinguishable particles.

In the case of bosons, field operators are analogous to the creation and annihilation operators for the electromagnetic field modes:

\[
\begin{align*}
\hat{b}^\dagger_\zeta |\phi\rangle & = \sqrt{n_\zeta + 1} |n_1, n_2, \ldots n_\zeta + 1, \ldots\rangle \\
\hat{b}_\zeta |\phi\rangle & = \sqrt{n_\zeta} |n_1, n_2, \ldots n_\zeta - 1, \ldots\rangle.
\end{align*}
\]

Although we will concentrate on bosons here, it is worth noting that the rules for raising and lowering fermion number are similar, but one must keep track of the negative signs which arise from anti-commutation.

One particularly useful basis is the momentum basis, \(|k\rangle\), with its associated creation and annihilation operators \(b_k\) and \(b^\dagger_k\). We can take the Fourier transform of these operators to define a real-space operator for the matter field

\[
\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_k e^{i\mathbf{k}\cdot\mathbf{r}} \hat{b}_k,
\]

Using the commutation relation, \([b_k, b^\dagger_{k0}] = \delta_{k,k0}\) we can find the commutation rules for:

\[
[\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')^\dagger] = \delta(\mathbf{r} - \mathbf{r}').
\]

Operators in the second quantization representation
Every atomic observable can be represented in terms of the matter field creation and annihilation operators. For example, the number operator is

\[ \hat{N} = \sum_\zeta \hat{b}_\zeta^\dagger \hat{b}_\zeta = \int d^3r \hat{\psi}(r)^\dagger \hat{\psi}(r). \]

\[ \hat{H} = \int d^3r \hat{\psi}(r)^\dagger \left( \frac{\hat{p}^2}{2m} + V_{\text{trap}}(r) \right) \hat{\psi}(r) + \frac{1}{2} \int d^3r \int d^3r' \hat{\psi}(r)^\dagger \hat{\psi}(r')^\dagger \hat{V}(r - r') \hat{\psi}(r') \hat{\psi}(r). \]

When the interatomic potential can be replaced by the s-wave pseudopotential, the second term can be considerably simplified, so that the Hamiltonian becomes

\[ \hat{H} = \int d^3r \hat{\psi}(r)^\dagger \left( \frac{\hat{p}^2}{2m} + V_{\text{trap}}(r) + \frac{U_0}{2} \hat{\psi}(r)^\dagger \hat{\psi}(r) \right) \hat{\psi}(r). \]

**Zero temperature non-interacting BEC**

It is instructive to consider the ground state at zero temperature in two types of potentials:

1. Homogeneous potential
2. Harmonic oscillator potential

The single particle states for these potentials are well known, and at zero temperature we expect all of the atoms to pile into the ground state. In the case of the infinite wall square well,

\[ \psi_0(r) \sim \sin \pi x/L \sin \pi y/L \sin \pi z/L. \]

The harmonic oscillator ground state wavefunction is a Gaussian

\[ \phi_0(r) = e^{-\left( \frac{x^2}{2a_x^2} + \frac{y^2}{2a_y^2} + \frac{z^2}{2a_z^2} \right)} \]

where \{a_x, a_y, a_z\} are the harmonic oscillator lengths associated with the trapping frequencies in each dimension.

If the atoms
do not interact, then the many-body state can be written as

$$|\Psi\rangle = (\hat{b}_0^\dagger)^N |\text{vac}\rangle,$$

where $b_0$ annihilates an atom in the ground state of the appropriate potential.

**Weak interactions: the Gross-Pitaevski equation**

If the interactions are sufficiently weak, then we qualitatively expect that Bose condensation should still occur, with most of the atoms occupying one quantum state. We now need to determine which state will be macroscopically occupied.

Using the Hamiltonian above, we can find the Heisenberg equations of motion for the matter field operator

$$i\hbar \frac{\partial}{\partial t} \psi = [\psi, \hat{H}] = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{trap}} + U_0 \hat{\psi}^\dagger \hat{\psi} \right) \psi.$$

This type of nonlinear operator equation is in general quite difficult to solve, but we can use our physical intuition to find an appropriate approximation.

In particular, since we expect macroscopic occupation of one state, the field operator should be close to a classical coherent field

$$\hat{\psi} = \psi + \delta \hat{\psi},$$

the Bose condensate can be well described by a classical nonlinear equation for $\psi$, known as the Gross-Pitaevski equation:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V_{\text{trap}} \psi + U_0 |\psi|^2 \psi.$$

The Gross-Pitaevski equation resembles a Schrodinger equation with a nonlinear term, where $\psi$ acts like the wavefunction for the Bose condensate. Since $\psi$ acts like a wavefunction, we should be careful about its normalization, which is set by the total number of particles.
\[ N = \int d^3 r |\psi|^2. \]

This normalization condition motivates us to interpret \( \psi \) as the condensate spatial density.

The Gross-Pitaevski equation provides an adequate description of most properties of zero temperature Bose condensates, and it bears a strong resemblance to the evolution of the electromagnetic field in a Kerr medium.

The relevant questions for a matter field, however, are rather different than those for light.

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**The ground state of a condensate at T=0**

The ground state of the electromagnetic field is the vacuum, but matter behaves rather differently because the total number of atoms is conserved, resulting in a finite chemical potential. The ground state is a stationary solution of the Gross-Pitaevski equation with phase evolution

\[ \psi = \tilde{\psi} e^{-i \mu t / \hbar}, \]

\[ \mu \tilde{\psi} = \left( -\frac{\hbar^2}{2m} \nabla^2 + V(r) + U_0 |\tilde{\psi}|^2 \right) \tilde{\psi}. \]

The character of the solution is determined by the relative importance of the kinetic energy terms and the interaction terms. The ratio of the trap frequency to the mean-field interaction energy \( E_{mf} \sim U_0 N / V \) is

\[ \frac{E_{mf}}{\hbar \omega_t} \approx \frac{4 \pi N a t^2}{V} \sim \frac{N a}{a_t}, \]

where \( a \) is the scattering length and \( a_t \) is the characteristic size of the harmonic oscillator trap. Note that the number of condensed atoms appears in the numerator of this expression, so even when the gas is weakly interacting \( (a \ll a_t) \) the interactions can still have important effects on the condensate behavior. When \( \hbar \omega_t > \)
$E_{mf}$, the condensate behaves essentially as a non-interacting gas. In the opposite limit $\hbar \omega_t < E_{mf}$ (known as the Thomas-Fermi regime for $U_0 > 0$) the interactions dominate.
The Thomas-Fermi approximation
When the interactions between atoms are strong and repulsive $U_0 > 0$, we can neglect the kinetic energy term. The resulting solution for the mean field is

$$|\tilde{\psi}|^2 = \begin{cases} \frac{\mu - V(r)}{U_0} & \text{for } r \text{ such that } V(r) < \mu \\ 0 & \text{for larger } r. \end{cases}$$

The chemical potential $\mu$ is set by the normalization condition

$$N = \int \frac{\mu - V(r)}{U_0} d^3r = N.$$

- For example, a BEC confined by a harmonic trap has a chemical potential given by

$$\mu = \frac{\hbar \omega_t}{2} \left( \frac{15Na}{a_t} \right)^{2/5}.$$

Since we are in the regime of strong interactions, the factor $Na/a_t$ increases the chemical potential significantly. The size of the condensate also increases due to interactions,

$$\bar{a} = a_t \left( \frac{15Na}{a_t} \right)^{\frac{2}{5}}.$$

This expansion makes physical sense because it lowers the energy cost of the repulsive interactions.

The healing length
The Thomas-Fermi approximation works poorly in regions where the atom density is insufficient to satisfy the assumption that the mean-field energy overwhelms kinetic energy. In particular, in the vicinity of the walls of the traps, the kinetic energy can no longer be neglected.
For example, consider a condensate in a box with infinite potential walls. The Thomas-Fermi approximation would predict that \( \psi = N/V \) is constant, dropping off suddenly to zero right at the edges of the box. Physically, this makes no sense: the wavefunction must be smooth even at the walls because sharp variations in \( \psi \) cause a high kinetic energy cost. We expect the wavefunction to fall off smoothly over some characteristic length \( \xi \). This so-called “healing length” can be estimated by equating the kinetic energy associated with variation on length \( \xi \) with the interaction energy \( \sim U_0 N/V \), which results in

\[
\xi^2 = \frac{1}{8\pi a N/V} = \frac{1}{8\pi n_0 a}.
\]

As long as the gas is sufficiently dilute \( na^3 \ll 1 \), the healing length extends over many atoms

\[
\xi \gg \frac{1}{n_0}.
\]

When this dilute gas assumption breaks down, the Gross-Pitaevski equation can no longer provide an adequate description of the condensate. We also note that the above discussion is valid only for repulsive atoms; we will find that problems arise for attractive interactions when the kinetic energy approaches the mean-field energy.