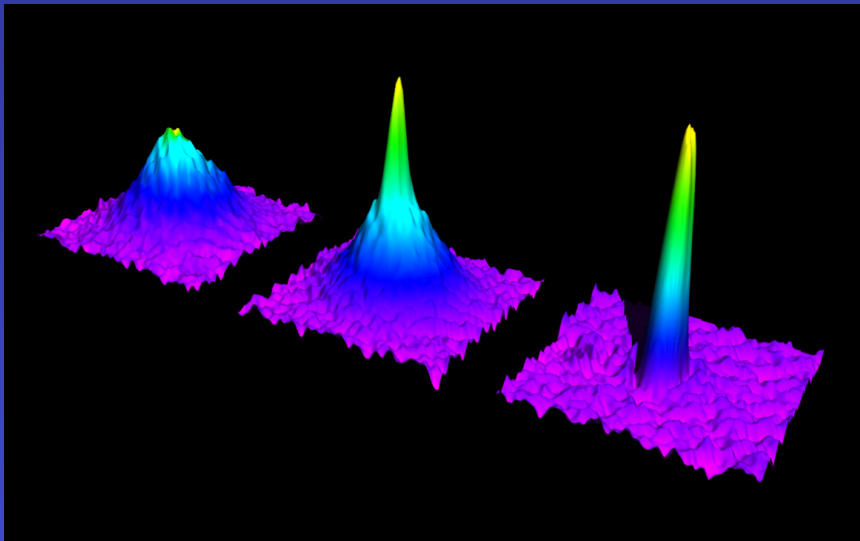


Dynamics of Bose-Einstein Condensates in Trapped Atomic Gases at Finite Temperature

Lecture 1: Basics

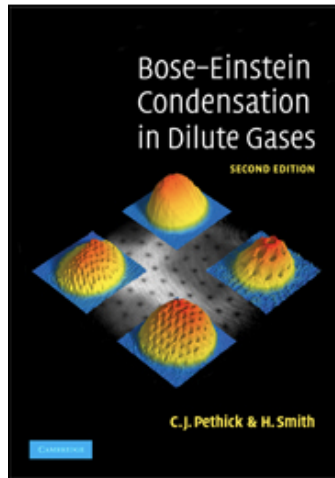
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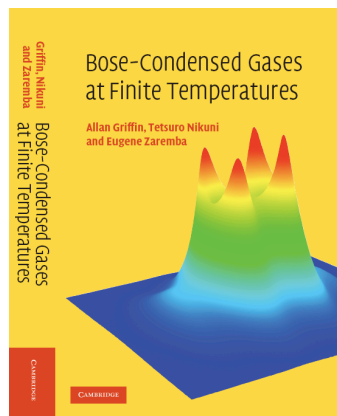
Main References



Bose-Einstein Condensation in Dilute Gases

C. J. Pethick and H. Smith

(Cambridge, 2008, second edition)



Bose-Condensed Gases at Finite Temperatures

A. Griffin, T. Nikuni and E. Zaremba

(Cambridge, 2009)

Main Collaborators

Allan Griffin, Tetsuro Nikuni and Brian Jackson

Outline of These Lectures

Lecture 1: Basics

- quantum statistics, ideal gases and Bose-Einstein condensation
- single-particle density matrix, Wigner distribution
- interactions in dilute gases
- Gross-Pitaevskii equation, Thomas-Fermi approximation
- Bose broken symmetry, order parameter
- time-dependent GP equation, quantum hydrodynamic equations, Stringari equation, Kohn theorem

Lecture 2: The ZNG Equations

- condensate wavefunction, the generalized GP equation, quantum hydrodynamics
- thermal component, Boltzmann kinetic equation, collisions
- equilibrium solution, equilibrium collision times
- condensate formation, adiabatic and ergodic approximations
- recap of ZNG equations

Outline, cont'd

Lecture 3: Solution of the ZNG Equations

- numerical solution of the GGP, split-operator method
- numerical solution of the kinetic equation, test-particle method, collision algorithm
- model of condensate growth
- the moment method, scissors mode and ZNG simulations
- the static thermal cloud approximation, dissipative GP equations

Lecture 4: Application of the ZNG Equations

- quadrupole modes: JILA and ENS experiments
- Landau damping: example of monopole (breathing) mode
- introduction to vortices
- stirring, rotating frames of reference
- vortex energetics
- phenomenological nucleation and equilibration of vortices
- ZNG simulations of vortex precession and relaxation

Trapped Atomic Gases

- a collection of particles confined by some potential
- this is a *many-body* system and I will be taking a *condensed matter physics* point of view in contrast to a quantum optics point of view; everything I will be talking about is most naturally described from this perspective
- these systems are inherently *quantum mechanical*. An isolated system can be described by a many-body wavefunction

$$\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$$

which evolves according to the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$$

Here H is the many-body Hamiltonian

$$H = \sum_{i=1}^N \left[\frac{p_i^2}{2m} + V_{\text{trap}}(\mathbf{r}_i, t) \right] + \sum_{i < j} v(|\mathbf{r}_i - \mathbf{r}_j|)$$

- in principle, if Ψ is known, all physical properties of the system can be determined. However, the direct determination of Ψ for a system with many particles is usually *impractical* (if not *impossible!*) and one must use physical insight in order to extract useful information.
- if the system is not isolated, a statistical description is necessary. Instead of being in a *pure state*, the quantum system is in a *mixture* of states. A good example of this is a system in thermal equilibrium. The system is represented by a *statistical ensemble* which is defined by means of a *density matrix*.

Q: Are trapped atomic gases isolated or not? If not, why not? Does it matter? If the gas is isolated, how does it ever get into thermal equilibrium?

Quantum Statistics

- the *indistinguishability* of *identical* particles plays a fundamental role in quantum mechanics

$|\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)|^2$ - probability of finding particle 1 at position \mathbf{r}_1 , particle 2 at \mathbf{r}_2 , etc.

$|\Psi(\mathbf{r}_2, \mathbf{r}_1, \dots, \mathbf{r}_N)|^2$ - probability of finding particle 1 at position \mathbf{r}_2 , particle 2 at \mathbf{r}_1 , etc.

- if the particles are identical, there is no way of distinguishing these probabilities, i.e., the probabilities must be the *same*. This implies the following *exchange symmetries*:

$$\Psi(\mathbf{r}_2, \mathbf{r}_1, \dots, \mathbf{r}_N) = \begin{cases} +\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \\ -\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \end{cases}$$

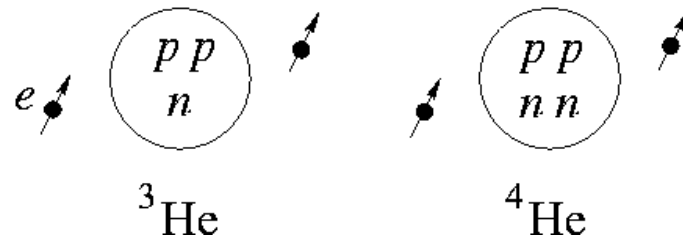
Q: Since we are talking about probabilities, isn't it possible to have an arbitrary phase $e^{i\alpha}$ in these relations? Then why \pm ?

Quantum Statistics, cont'd

- one observes in nature that the symmetric wavefunctions (+) are associated with particles with integral spin: *bosons*
- particles with half-integral spin (−) are associated with antisymmetric wavefunctions: *fermions*
- composite particles (atoms) also obey quantum statistics; the simple rule is that atoms composed of an *odd* number of elementary fermions (electrons, protons, neutrons) are themselves *fermions*. On the other hand, if one has an *even* number of fermions, the atom behaves as a *boson*.

At the microscopic level, the classification of particles is based on the behaviour of the many-body wave function under the exchange of identical particles.

Quantum Statistics, an example



- both isotopes are chemically equivalent and have (essentially) the *same* atomic spectra (*Q: Why would the spectra differ at all?*)
- however, in liquid form at low temperatures, they behave *completely differently!*
- ${}^4\text{He}$ becomes a *superfluid* below $T \sim 2$ K while ${}^3\text{He}$ is a *viscous liquid*, before finally becoming a (different kind of) superfluid below $T \sim 2$ mK
- in both cases, these properties are associated with the phenomenon of *Bose-Einstein condensation*

Ideal Gases

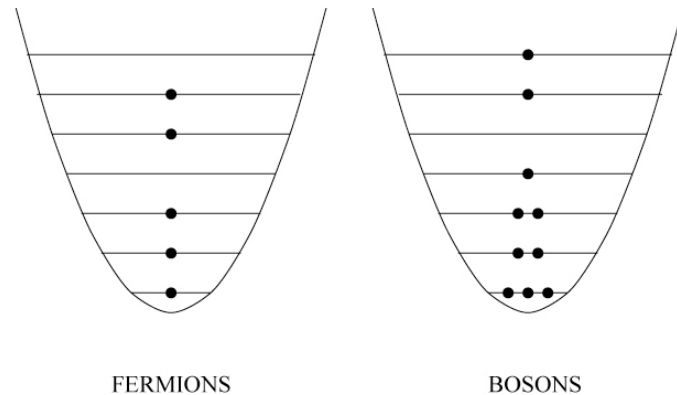
- idealization of no interparticle interactions
- many-body quantum states can be built out of single-particle wavefunctions

$$h = -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{trap}}(\mathbf{r}); \quad h\phi_\alpha = \epsilon_\alpha \phi_\alpha$$

- case of 2 particles

$$\Psi_{\text{B/F}}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} [\phi_\alpha(\mathbf{r}_1)\phi_\beta(\mathbf{r}_2) \pm \phi_\alpha(\mathbf{r}_2)\phi_\beta(\mathbf{r}_1)]$$

- if $\alpha = \beta$, the fermionic wavefunction vanishes: *Pauli exclusion principle*; there is no such restriction for bosons
- quantum statistics has a profound effect on the occupancy of single-particle states; in particular, the ground state of a bosonic system has all the particles in the *lowest quantum state*



Ideal Gases, Many-Particle States

- a convenient basis of many-particle states is provided by the *occupation number representation*

$|\{n_\alpha\}\rangle$ - $\{n_\alpha\}$ is a set of integers giving the number of particles in each of the states α

$$n_\alpha = \begin{cases} 0, 1 & \text{for fermions} \\ 0, 1, \dots, \infty & \text{for bosons} \end{cases}$$

- the algebra of creation and annihilation operators facilitates working with properly symmetrized states. For bosons we have

$$\begin{aligned} \hat{a}_\alpha |n_1, n_2, \dots, n_\alpha, \dots\rangle &= \sqrt{n_\alpha} |n_1, n_2, \dots, n_\alpha - 1, \dots\rangle \\ \hat{a}_\alpha^\dagger |n_1, n_2, \dots, n_\alpha, \dots\rangle &= \sqrt{n_\alpha + 1} |n_1, n_2, \dots, n_\alpha + 1, \dots\rangle \\ [\hat{a}_\alpha, \hat{a}_\beta^\dagger] &= \delta_{\alpha\beta}, \quad [\hat{a}_\alpha, \hat{a}_\beta] = 0, \quad [\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger] = 0 \end{aligned}$$

- all operators can be expressed in a *second-quantized* form:

$$\begin{aligned} H_0 &= \sum_{\alpha\beta} \langle \alpha | h | \beta \rangle \hat{a}_\alpha^\dagger \hat{a}_\beta, \quad H_0 |\{n_\alpha\}\rangle = E_0(\{n_\alpha\}) |\{n_\alpha\}\rangle \\ E_0(\{n_\alpha\}) &= \sum_{\alpha} \epsilon_\alpha n_\alpha, \quad N(\{n_\alpha\}) = \sum_{\alpha} n_\alpha \end{aligned}$$

Ideal Gases, Thermal Properties

- the state of thermal equilibrium can be represented by the *grand canonical ensemble* with density matrix

$$\hat{\rho}_0 = \frac{1}{Z} e^{-\beta(\hat{H}_0 - \mu\hat{N})}, \quad Z = \text{Tr} e^{-\beta(\hat{H}_0 - \mu\hat{N})} = \sum_{\{n_\alpha\}} e^{-\beta[E_0(\{n_\alpha\}) - \mu N(\{n_\alpha\})]}$$

- thermal averages are then given by

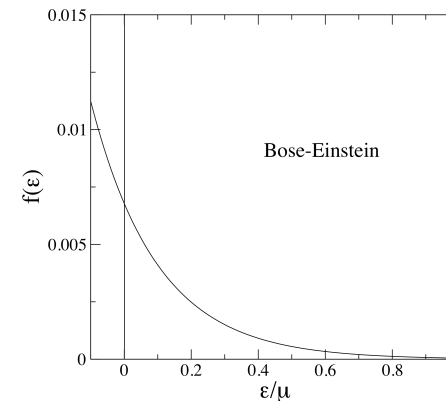
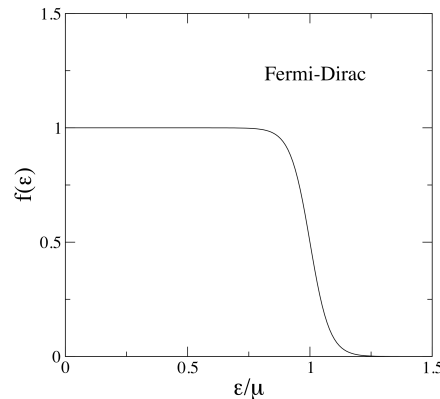
$$\langle \hat{O} \rangle = \text{Tr} (\hat{\rho}_0 \hat{O})$$

- in particular, the average occupation of a state α is given by

$$\langle \hat{n}_\alpha \rangle = \frac{1}{e^{\beta(\epsilon_\alpha - \mu)} \pm 1} \quad \text{fermions (+), bosons (-)}$$

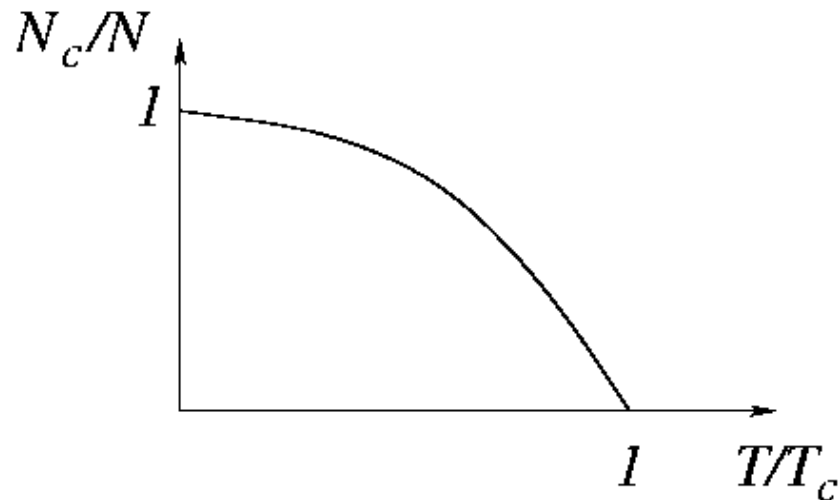
E: If you've never done so, derive this result!

$$f(\epsilon) = \frac{1}{e^{\beta(\epsilon - \mu)} \pm 1}$$



Bose-Einstein Condensation

- in 1924 (published in 1925), Einstein predicted a novel kind of condensation in a gas of *noninteracting* bosons
- he considered N particles in a box of volume V and reasoned that the number of particles in the lowest quantum state ($p = 0$) would suddenly increase below a certain critical temperature, T_c , i.e., a *finite fraction* of all the particles would suddenly find themselves in the *lowest* available quantum state:



- at $T = 0$, *all* particles are in the lowest quantum state; this is the *ground state* of the system

BEC, more quantitatively

- the BE distribution function determines the average number of particles in the box:

$$\langle N \rangle = \sum_{\mathbf{p}} \frac{1}{e^{\beta(\epsilon_{\mathbf{p}} - \mu)} - 1} \rightarrow V \int \frac{d^3p}{(2\pi\hbar)^3} \frac{1}{e^{\beta(\epsilon_{\mathbf{p}} - \mu)} - 1}$$

- for a fixed temperature, $\langle N \rangle$ is a monotonically increasing function of μ , reaching its maximum at $\mu = 0$

$$N_{\max}(T) = V \int \frac{d^3p}{(2\pi\hbar)^3} \frac{1}{e^{\beta\epsilon_{\mathbf{p}}} - 1} = V \left(\frac{m}{2\pi\beta\hbar^2} \right)^{3/2} g_{3/2}(1) \quad g_n(x) = \sum_{k=1}^{\infty} \frac{x^k}{k^n}$$

$$g_{3/2}(1) = 2.612$$

- it would seem that $N \leq N_{\max}(T)$; but N is a variable at our disposal. The condition $N = N_{\max}(T_c)$ defines the transition temperature

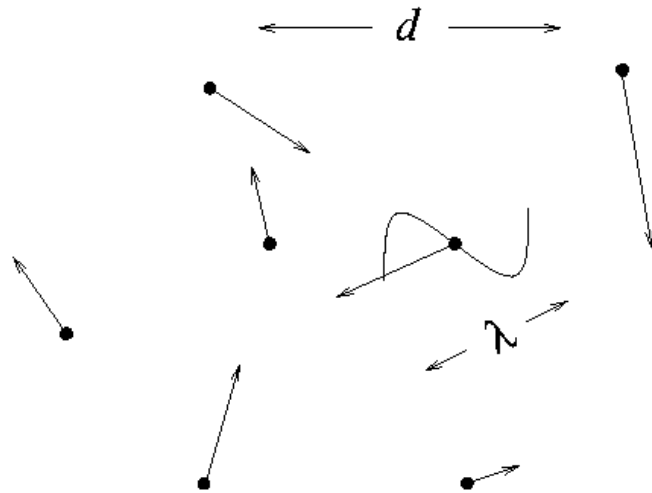
$$T_c = \left(\frac{2\pi\hbar^2}{mk_B} \right) \frac{n^{3/2}}{[g_{3/2}(1)]^{3/2}}$$

- for $T < T_c$, $N_{\max}(T) < N$. A finite number $N_0 = N - N_{\max}(T)$ of the atoms *must* then be placed in the $p = 0$ state:

$$N_0 = N \left[1 - \left(\frac{T}{T_c} \right)^{3/2} \right]$$

BEC, physically

- BEC is a consequence of *quantum degeneracy*



- d , mean spacing between atoms in the gas; $n \sim d^{-3}$
- the thermal de Broglie wavelength is

$$\lambda_T = \sqrt{\frac{2\pi\hbar^2}{mk_B T}}$$

- the criterion for quantum degeneracy is

$$\lambda_T \sim d \Rightarrow T_c \simeq \frac{h^2 n^{3/2}}{mk_B}$$

E: Show that BEC does not occur for a 1D or 2D gas. What is the physical reason for this? Yet in 0D (a trapped Bose gas) we will find that there is a BEC transition! Think about this (later) and explain why this is happening. Note that in all cases, the ground state has all particles in the lowest energy quantum state.

Achieving BEC in Trapped Atomic Gases

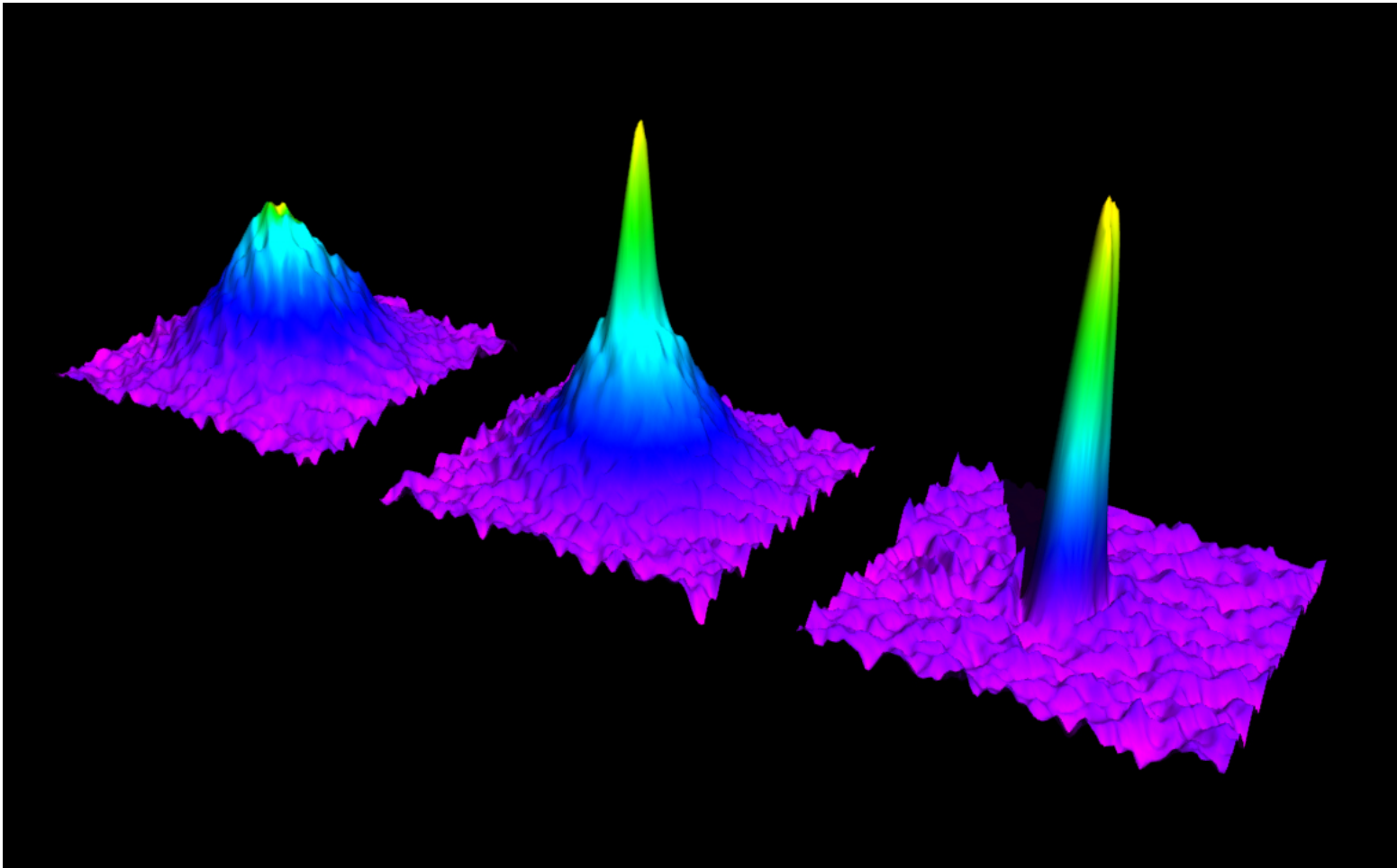
- the one naturally occurring Bose liquid is ^4He , however in this case, the interactions between the atoms are strong and the effects of Bose-Einstein condensation are obscured
- for this reason, there was considerable interest in finding other systems in which BEC might occur; of course there was nothing stopping theorists (e.g. Bogoliubov) from studying *weakly* interacting Bose gases!
- work began in the early 1970's to achieve BEC in a gas of spin-polarized hydrogen; achieved in 1999
- however, a parallel effort to achieve BEC in gases of alkali atoms began in the early 1990's and in fact succeeded in 1995!
- the Nobel prize in physics was awarded in 2001 to Eric Cornell, Carl Wieman and Wolfgang Ketterle for this achievement

Experimental Challenges

There were many technical challenges that had to be overcome in order to achieve BEC in trapped gases:

- the gas has to be *dilute* in order to prevent the atoms from condensing into a *solid*
- a method is needed for *slowing* thermal atoms down sufficiently in order for them to be trapped
- a method for *holding* a gas of atoms in place must be devised
- and once the atoms are trapped, they must be *cooled* to sufficiently low temperatures in order for BEC to occur
- once these techniques had been mastered, experimentalists found...

...BEC in a Trapped Gas!



Ideal Gas in Harmonic Traps

- we consider a general anisotropic harmonic trap

$$V_{\text{trap}}(\mathbf{r}) = \frac{1}{2}m\omega_x^2x^2 + \frac{1}{2}m\omega_y^2y^2 + \frac{1}{2}m\omega_z^2z^2$$

- the single-particle states are

$$\phi_{n_x n_y n_z}(x, y, z) = X_{n_x}(x)Y_{n_y}(y)Z_{n_z}(z) \quad n_i = 0, 1, \dots, \infty$$

with energies

$$E_{n_x n_y n_z} = \left(n_x + \frac{1}{2}\right) \hbar\omega_x + \left(n_y + \frac{1}{2}\right) \hbar\omega_y + \left(n_z + \frac{1}{2}\right) \hbar\omega_z$$

- characteristic lengths are defined by

$$\omega_{ho} = (\omega_x\omega_y\omega_z)^{1/3}, \quad a_i = \sqrt{\frac{\hbar}{m\omega_i}}, \quad a_{ho} = \sqrt{\frac{\hbar}{m\omega_{ho}}}$$

- number of particles in the ground and excited states are

$$N_0 = \frac{1}{e^{\beta(E_{000}-\mu)} - 1}, \quad \tilde{N} = \sum'_{n_x n_y n_z} \frac{1}{e^{\beta(E_{n_x n_y n_z}-\mu)} - 1}$$

- maximum number of particles in excited states is

$$\tilde{N}_{max} = \sum'_{n_x n_y n_z} \frac{1}{e^{\beta(E_{n_x n_y n_z}-E_{000})} - 1} \simeq \int_0^\infty dn_x \int_0^\infty dn_y \int_0^\infty dn_z \frac{1}{e^{\beta\hbar(n_x\omega_x+n_y\omega_y+n_z\omega_z)} - 1}$$

Ideal Gas in Harmonic Traps, cont'd

- one finds

$$\tilde{N}_{max}(T) = \left(\frac{k_B T}{\hbar \omega_{ho}} \right)^3 \zeta(3), \quad \zeta(3) = 1.202\dots$$

E: Derive this result.

- the critical temperature is then defined by

$$N_{max}(T_c) = N \Rightarrow k_B T_c = \hbar \omega_{ho} \left(\frac{N}{\zeta(3)} \right)^{1/3}$$

and for $T < T_c$, we find

$$N_0(T) = N \left[1 - \left(\frac{T}{T_c} \right)^3 \right]$$

E: Show classically that the cloud has an extent given by $R_i = (2k_B T / m \omega_i^2)^{1/2}$ in the i -direction. Then show that the criterion $\lambda_T \approx d$ gives a critical temperature consistent with the expression above. Compare the extent of the cloud at T_c with the harmonic oscillator length a_{ho} .

E: Show that the transition temperature for a gas confined by a two-dimensional harmonic potential is $k_B T_c^{2D} = \hbar \omega_{ho} (6N/\pi^2)^{1/2}$.

The Single-Particle Density Matrix

- as we shall see, the single-particle density matrix plays an important role for a Bose-condensed system. For an N -particle state $|\Psi\rangle$, it is defined as

$$\begin{aligned}\rho(\mathbf{r}, \mathbf{r}') &= N \int d\mathbf{r}_2 \dots d\mathbf{r}_N \Psi^*(\mathbf{r}', \mathbf{r}_2, \dots, \mathbf{r}_N) \Psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) \\ &= \langle \Psi | \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}) | \Psi \rangle, \quad [\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}')\end{aligned}$$

E: Prove the equivalence of these definitions.

- for an ensemble of states we have $\rho_1(\mathbf{r}, \mathbf{r}') = \langle \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}) \rangle$
- the diagonal component $\rho_1(\mathbf{r}, \mathbf{r})$ is the number density $n(\mathbf{r})$ and

$$\langle \hat{N} \rangle = \int d^3r \rho_1(\mathbf{r}, \mathbf{r})$$

- the single-particle density matrix is a *Hermitian operator*, $\rho_1^*(\mathbf{r}, \mathbf{r}') = \rho_1(\mathbf{r}', \mathbf{r})$; it has eigenfunctions and eigenvalues defined by

$$\int d^3r' \rho_1(\mathbf{r}, \mathbf{r}') \phi_i(\mathbf{r}') = n_i \phi_i(\mathbf{r})$$

- the eigenfunctions form an orthonormal set and the eigenvalues are real

Wigner Operator

- we now define the *Wigner operator*

$$\hat{f}(\mathbf{p}, \mathbf{r}) \equiv \int d^3r' e^{i\mathbf{p}\cdot\mathbf{r}'/\hbar} \hat{\psi}^\dagger(\mathbf{r} + \frac{1}{2}\mathbf{r}') \hat{\psi}(\mathbf{r} - \frac{1}{2}\mathbf{r}')$$

- it is easy to show that the number density operator is given by

$$\hat{n}(\mathbf{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} \hat{f}(\mathbf{p}, \mathbf{r})$$

- now introduce the Fourier transform of the field operator

$$\hat{\phi}(\mathbf{p}) = \int \frac{d^3r}{(2\pi\hbar)^{3/2}} e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \hat{\psi}(\mathbf{r})$$

$$[\hat{\phi}(\mathbf{p}), \hat{\phi}^\dagger(\mathbf{p}')] = \delta(\mathbf{p} - \mathbf{p}')$$

- the momentum space density operator is given by

$$\hat{v}(\mathbf{p}) = \int \frac{d^3r}{(2\pi\hbar)^3} \hat{f}(\mathbf{p}, \mathbf{r}) \quad (E: \text{Prove this result.})$$

- the *expectation value* of the Wigner operator thus has the properties of a *phase space distribution function*. This function, however, is not positive definite in general and thus cannot be interpreted strictly as a probability density.

Equation of Motion for the Wigner Distribution

- in the Heisenberg picture, the time evolution of an operator is given by

$$i\hbar \frac{d\hat{O}(t)}{dt} = [\hat{O}(t), \hat{H}], \quad \hat{O}(t) = e^{i\hat{H}t/\hbar} \hat{O} e^{-i\hat{H}t/\hbar}$$

- for the case of noninteracting particles, the Wigner distribution function can be shown to satisfy the equation

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{r}} f - \nabla_{\mathbf{r}} V \cdot \nabla_{\mathbf{p}} f = -\frac{\hbar^2}{24} h(\mathbf{r}, \mathbf{p}) \left(\overleftarrow{\nabla}_{\mathbf{r}} \cdot \overrightarrow{\nabla}_{\mathbf{p}} \right)^3 f + O(\hbar^4)$$

where h is the single-particle classical Hamiltonian

$$h(\mathbf{r}, \mathbf{p}) = \frac{p^2}{2m} + V(\mathbf{r})$$

- the left-hand side is called the *free-streaming term* and is purely a classical result; the right-hand side shows the quantum corrections developed as a series in powers of Planck's constant \hbar . To lowest order, the equilibrium distribution function is simply

$$f_0(h(\mathbf{r}, \mathbf{p})) = \frac{1}{e^{\beta(p^2/2m + V(\mathbf{r}) - \mu)} - 1}$$

- I will refer to this as the *semiclassical* Bose-Einstein distribution function.

Harmonic Trap in the Semiclassical Approximation

- the number of particles in the trap is given by

$$\tilde{N} = \int \frac{d^3r d^3p}{(2\pi\hbar)^3} \frac{1}{\exp[\beta(p^2/2m + (m/2)(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) - \mu)] - 1}$$

- this number is maximized for $\mu = 0$ and we find

$$\begin{aligned}\tilde{N}_{max}(T) &= \left(\frac{k_B T}{\pi\hbar\omega_{ho}}\right)^3 \int d^6x \frac{1}{\exp(x_1^2 + \dots + x_6^2) - 1} \\ &= \left(\frac{k_B T}{\hbar\omega_{ho}}\right)^3 \zeta(3)\end{aligned}$$

E: Prove this result. Hint: Determine the volume of a 6-dimensional sphere.

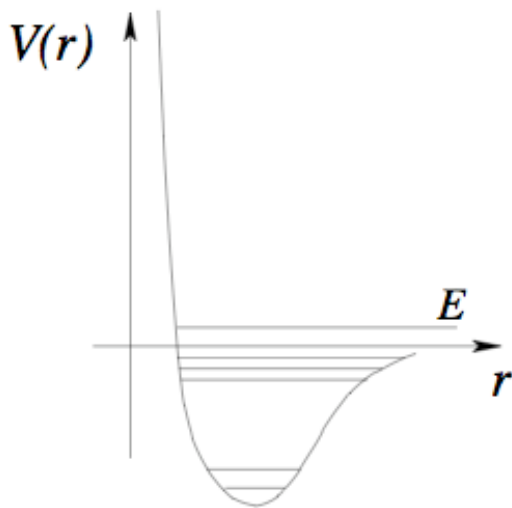
- the above is the same result obtained earlier and leads to the conclusion that the number of condensate atoms for $T < T_c$ is

$$N_0(T) = N \left[1 - \left(\frac{T}{T_c}\right)^3 \right]$$

- we see that this result can be viewed as being a consequence of the semiclassical approximation to the Wigner distribution function; but this function also provides an expression for the *density* in the trap

Interactions

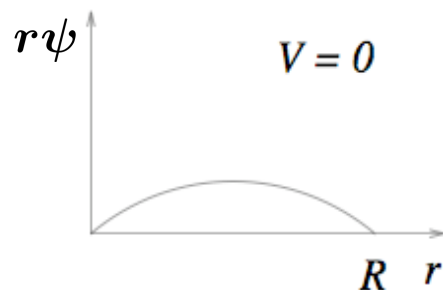
- even though the gas is dilute, interactions between the atoms still play an important role. But in dilute gases, interactions are included in a special way.



- to the left is a sketch of a conventional interatomic potential. It supports several molecular bound states. To access these bound states requires at least a *3-body collision*, but these are rare in a dilute gas. Thus, although a dilute gas is in principle *metastable*, it is effectively stable on the time-scale of typical experiments. The system we are dealing with is thus an ensemble of cold atoms undergoing binary collisions. However, ‘collisions’ mean something more in a degenerate Bose gas!

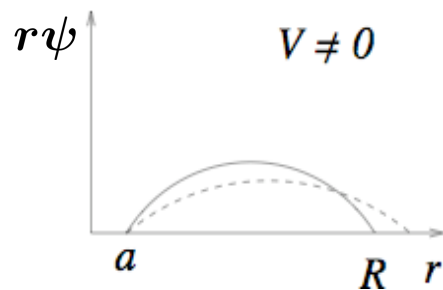
Interactions, cont'd

- consider a pair of atoms in a spherical box of radius R . The relative wavefunction is sketched below for two situations, with and without the interatomic potential.



- for $V = 0$, we require the wavefunction to vanish at the boundary ($r = R$). The pair of atoms thus has an energy

$$E = \frac{\hbar^2 k^2}{2\mu} = \frac{\hbar^2}{2\mu} \left(\frac{\pi}{R} \right)^2$$



- for $V \neq 0$, the wavefunction *at this energy* will look something like the dashed line in the figure in the asymptotic region where the wavefunction behaves as

$$r\psi(r) \sim \sin k(r - a)$$

- here, a is the s -wave scattering length which can be either positive or negative; if the wavefunction is to fit in the box, we must change k

$$k \Rightarrow k' = \frac{\pi}{R - a} \simeq \frac{\pi}{R} + \frac{\pi a}{R^2}$$

Interactions, cont'd

- the change in energy of the state is thus

$$\Delta E = E' - E = \frac{\hbar^2 k'^2}{2\mu} - \frac{\hbar^2 k^2}{2\mu} \simeq \frac{\pi^2 a \hbar^2}{m R^3}$$

- if we multiply this by the number of atoms in the gas, we have

$$\Delta E \sim \frac{a \hbar^2}{m} n$$

- this is effectively the energy required to place an atom into a gas of density n ; when done more carefully, the interaction between atoms can be represented by the *pseudopotential*

$$U(r) = \frac{4\pi a \hbar^2}{m} \delta(r) \equiv g \delta(r)$$

- if a is positive (negative) the effective interaction is repulsive (attractive); interestingly, this ‘interaction’ is associated with a change in kinetic energy of the gas! This short-ranged potential can be used as the effective interaction but care must be exercised when doing so.

$$\hat{H}_{int} = \frac{g}{2} \int d^3 r \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r})$$

Variational Ground State of the Interacting Gas

- the complete second-quantized Hamiltonian is

$$\hat{H} = \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{trap}}(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) + \frac{g}{2} \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r})$$

- let's expand the field operator in a single-particle basis (e.g. trap states)

$$\hat{\psi}(\mathbf{r}) = \sum_i \phi_i(\mathbf{r}) \hat{a}_i$$

and consider the *variational ground state*

$$|\Psi\rangle = |N, 0, 0, \dots\rangle$$

- this state has all the particles in a *single* quantum state $\phi_0(\mathbf{r})$; we then have

$$E[\phi_0] \equiv \langle \Psi | \hat{H} | \Psi \rangle = N \int d^3r \phi_0^*(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{trap}}(\mathbf{r}) \right] \phi_0(\mathbf{r}) + \frac{1}{2} N(N-1) \int d^3r |\phi_0(\mathbf{r})|^4$$

- this must now be minimized with respect to $\phi_0(\mathbf{r})$; the normalization constraint is achieved by means of a Lagrange parameter and we then minimize freely

$$K[\phi_0] = N \int d^3r \phi_0^*(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{trap}}(\mathbf{r}) \right] \phi_0(\mathbf{r}) + \frac{1}{2} N(N-1) \int d^3r |\phi_0(\mathbf{r})|^4 - \mu_0 N \int d^3r |\phi_0(\mathbf{r})|^2$$

The Time-independent Gross-Pitaevskii Equation

- in this way we arrive at the celebrated *Gross-Pitaevskii* equation

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{trap}}(\mathbf{r}) + g|\Phi_0(\mathbf{r})|^2 \right] \Phi_0(\mathbf{r}) = \mu_0 \Phi_0(\mathbf{r})$$

where the *condensate wavefunction* is

$$\Phi_0(\mathbf{r}) = \sqrt{N} \phi_0(\mathbf{r})$$

E: Show that the variation of K leads to the GP equation.

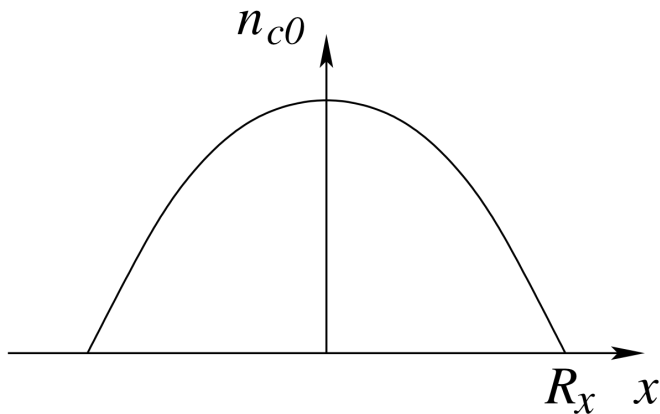
- because of the interactions, the GP equation is *nonlinear* and the usual properties of the linear Schrödinger equation no longer apply; this state is the closest one can come in an interacting Bose gas to putting all the particles into the ‘lowest quantum state’
- the nonlinearity of the GP equation typically requires an *iterative* procedure in order to obtain its solutions
- the ‘ground’ state is not the only state of physical interest; *‘excited’* states are also accessible experimentally
- as we shall see, there is also a *dynamical* version of this equation

The Thomas-Fermi Approximation

- it is *not* straightforward to solve the nonlinear GP equation; there is however a remarkably simple and accurate solution when the number of particles is *large*
- neglecting the kinetic energy term in the GP equation we obtain

$$n_{c0}(\mathbf{r}) = \frac{1}{g} [\mu_0 - V_{\text{trap}}(\mathbf{r})]$$

- this is an explicit expression for the condensate density $n_{c0}(\mathbf{r}) = |\Phi_0(\mathbf{r})|^2$ which is valid when $\mu_0 < V_{\text{trap}}(\mathbf{r})$; for a harmonic trap, the density profile is an *inverted parabola*; the chemical potential μ_0 controls the number of particles N in the trap



- the TF radius is given by

$$R_x = \sqrt{2\mu_0/m\omega_x^2}$$

- the approximation is valid if

$$R_x \gg a_x$$

- the approximation breaks down at the edge of the condensate

So, what exactly is the condensate wavefunction?

- at first sight the condensate wavefunction may seem rather mysterious
- the single-particle density matrix provides some insight. Recall

$$\rho_1(\mathbf{r}, \mathbf{r}') = \langle \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}) \rangle$$
$$\int d^3r' \rho_1(\mathbf{r}, \mathbf{r}') \phi_i(\mathbf{r}') = n_i \phi_i(\mathbf{r})$$

- in terms of these eigenfunctions – *natural orbitals* – we have

$$\rho_1(\mathbf{r}, \mathbf{r}') = \sum_i n_i \phi_i^*(\mathbf{r}') \phi_i(\mathbf{r}), \quad n(\mathbf{r}) = \rho_1(\mathbf{r}, \mathbf{r}) = \sum_i n_i |\phi_i(\mathbf{r})|^2$$

- the total number of particles is thus given by

$$N = \sum_i n_i = n_0 + \sum_{i \neq 0} n_i$$

That is, the eigenvalues can be interpreted as the *occupation numbers* of the natural orbitals; we have isolated the largest eigenvalue n_0 . For a Bose-condensed system, this eigenvalue will be of order N . We say that the corresponding orbital is *macroscopically occupied*.

OK, now we're beginning to see what it means!

- defining $\Phi_0(\mathbf{r}) = \sqrt{n_0}\phi_0(\mathbf{r})$ we have

$$\rho_1(\mathbf{r}, \mathbf{r}') = \Phi_0^*(\mathbf{r}')\Phi_0(\mathbf{r}) + \sum_{i \neq 0} n_i \phi_i^*(\mathbf{r}')\phi_i(\mathbf{r})$$

- if we now suppose that (Bogoliubov, 1947)

$$\langle \hat{\psi}(\mathbf{r}) \rangle = \Phi_0(\mathbf{r}), \quad \hat{\psi}(\mathbf{r}) \equiv \Phi_0(\mathbf{r}) + \tilde{\psi}(\mathbf{r}), \quad \langle \tilde{\psi}(\mathbf{r}) \rangle = 0$$

we have

$$\rho_1(\mathbf{r}, \mathbf{r}') = \Phi_0^*(\mathbf{r}')\Phi_0(\mathbf{r}) + \langle \tilde{\psi}^\dagger(\mathbf{r}')\tilde{\psi}(\mathbf{r}) \rangle$$

- in other words, the assumption of *Bose broken symmetry* reproduces the form of the single particle density matrix. The expectation value of the field operator plays the role of the *order parameter* for the Bose superfluid phase transition:

$$\Phi_0(\mathbf{r}) = \begin{cases} 0, & \text{if } T > T_{\text{BEC}} \\ \neq 0, & \text{if } T < T_{\text{BEC}} \end{cases}$$

- note in general that

$$\int d^3r |\Phi_0(\mathbf{r})|^2 = n_0 \neq N$$

- in an interacting system this is true even at $T = 0$: *quantum depletion*

Bose Broken Symmetry

- of course in a conventional average involving states with a *definite number of particles* we must have

$$\langle \hat{\psi}(\mathbf{r}) \rangle = 0$$

- so in what sense can this average be nonzero? If we imagine introducing into the Hamiltonian a symmetry breaking perturbation

$$\hat{H}_{\text{SB}} = \int d\mathbf{r} \left[\eta(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) + \eta^*(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right]$$

the Hamiltonian is no longer number-conserving and the field operator can have a finite average. If we then find

$$\lim_{\eta \rightarrow 0} \langle \hat{\psi}(\mathbf{r}) \rangle = \Phi_0(\mathbf{r}) \neq 0$$

we can say that the system is *Bose-condensed*. This is analogous to what is done for a magnetic phase transition – there we introduce a weak magnetic field which breaks the *isotropy* of space, thereby allowing the magnetization to point in a given direction. Here the symmetry-breaking perturbation fixes the *phase* of the order parameter. When all is said and done, we can simply assume in the theory that $\langle \hat{\psi}(\mathbf{r}) \rangle \neq 0$ for a Bose-condensed system.

The Time-dependent GP equation

- if we are not dealing with an equilibrium situation, the order parameter will be *time-dependent*. The condensate wavefunction is then described by the time-dependent GP equation

$$i\hbar \frac{\partial \Phi(\mathbf{r}, t)}{\partial t} = \left[-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{trap}}(\mathbf{r}) + g|\Phi(\mathbf{r}, t)|^2 \right] \Phi(\mathbf{r}, t)$$

- this equation seems an obvious generalization of the time-independent GP equation but I will not justify it at this point since a detailed derivation will be provided in Lecture 2. The point is that this equation can describe the dynamics of the condensate at $T = 0$. In particular, it can be used to study the *collective modes* of the condensate, or the *normal modes of oscillation*. I want to illustrate this with a few examples.
- first, let's reformulate the TDGP equation using the amplitude-phase representation of the condensate wavefunction:

$$\Phi(\mathbf{r}, t) = \sqrt{n_c(\mathbf{r}, t)} e^{i\theta(\mathbf{r}, t)}$$

The Time-dependent GP equation, cont'd

- substituting this into the TDGP equation, the left hand side is

$$\frac{i\hbar}{\Phi} \frac{\partial \Phi}{\partial t} = -\hbar \frac{\partial \theta}{\partial t} + \frac{i\hbar}{2n_c} \frac{\partial n_c}{\partial t}$$

and the right hand side becomes

$$\begin{aligned} \frac{1}{\Phi} \left(-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{trap}} + gn_c \right) \Phi = & -\frac{\hbar^2}{2m} \frac{\nabla^2 \sqrt{n_c}}{\sqrt{n_c}} + \frac{\hbar^2}{2m} |\nabla \theta|^2 + V_{\text{trap}} + gn_c \\ & - \frac{i\hbar^2}{2mn_c} (\nabla n_c \cdot \nabla \theta + n_c \nabla^2 \theta) \end{aligned}$$

- equating real and imaginary parts of these equations, we arrive at

$$\frac{\partial n_c}{\partial t} + \nabla \cdot (n_c \mathbf{v}_c) = 0$$

$$m \frac{\partial \mathbf{v}_c}{\partial t} = -\nabla \left(\mu_c + \frac{1}{2} m v_c^2 \right)$$

with

$$\mu_c(\mathbf{r}, t) \equiv -\frac{\hbar^2 \nabla^2 \sqrt{n_c(\mathbf{r}, t)}}{2m \sqrt{n_c(\mathbf{r}, t)}} + V_{\text{trap}}(\mathbf{r}) + gn_c(\mathbf{r}, t), \quad \mathbf{v}_c(\mathbf{r}, t) \equiv \frac{\hbar}{m} \nabla \theta(\mathbf{r}, t)$$

E: Derive these equations.

The Time-dependent GP equation, cont'd

- we have thus reduced the TDGP equation to two coupled equations in the *'hydrodynamic'* variables n_c and \mathbf{v}_c which are similar to the hydrodynamic equations for a normal fluid.
- the dynamic TF approximation neglects the *'quantum pressure'* term in the chemical potential. The equations can be linearized by introducing

$$\begin{aligned}n_c &= n_{c0} + \delta n_c \\ \mathbf{v}_c &= \mathbf{v}_{c0} + \delta \mathbf{v}_c\end{aligned}$$

- assuming $\mathbf{v}_{c0} = 0$, we obtain the Stringari equation (1996)

$$\frac{\partial^2 \delta n_c(\mathbf{r}, t)}{\partial t^2} = \frac{g}{m} \nabla \cdot [n_{c0}(\mathbf{r}) \nabla \delta n_c(\mathbf{r}, t)]$$

E: Derive this equation.

- this equation was first derived by Stringari in 1996. It has been very useful in the study of the collective modes in a pure condensate at $T = 0$: more about this in Lecture 3.

Sound Waves in a Uniform Condensate

- in a uniform Bose gas (no trapping potential) the normal mode solutions are plane waves

$$\delta n_c(\mathbf{r}, t) = \delta n_{\mathbf{q}\omega} e^{i(\mathbf{q}\cdot\mathbf{r} - \omega t)}$$

- substituting this into the Stringari equation we obtain

$$-\omega^2 \delta n_{\mathbf{q}\omega} = \frac{gn_{c0}}{m} (-q^2) \delta n_{\mathbf{q}\omega}$$

with the solution

$$\omega^2 = c_0^2 q^2$$

- the collective mode is a *phonon-like* excitation with a sound speed of

$$c_0 = \sqrt{gn_{c0}/m}$$

- if the quantum pressure term is retained, the excitation frequency is given by the Bogoliubov result (also see Lecture 3)

$$\hbar\omega = (\varepsilon_q^2 + 2gn_{c0}\varepsilon_q)^{1/2}, \quad \varepsilon_q = \frac{\hbar^2 q^2}{2m}$$

E: Obtain this result by retaining and linearizing the quantum pressure term in the hydrodynamic equations.

The Kohn Theorem

- to conclude this first lecture let's obtain an important result for atoms confined by a harmonic potential. This result was first established by Kohn (1961) in the context of the cyclotron resonance in metals and extended to harmonically-confined electrons by Dobson (1994).
- assume the Hamiltonian

$$H = \sum_{i=1}^N \left[\frac{p_i^2}{2m} + \frac{1}{2}m(\omega_x^2 x_i^2 + \omega_y^2 y_i^2 + \omega_z^2 z_i^2) \right] + \sum_{i<j} v(|\mathbf{r}_i - \mathbf{r}_j|)$$

and define the centre-of-mass position operator

$$\hat{R}_\alpha = \frac{1}{N} \sum_{i=1}^N r_{i\alpha}$$

- the Heisenberg equation of motion for this operator is

$$\frac{d\hat{R}_\alpha}{dt} = \frac{1}{i\hbar} [\hat{R}_\alpha, H] = \frac{\hat{P}_\alpha}{M}, \quad \hat{P}_\alpha \equiv \sum_{i=1}^N p_{i\alpha}, \quad M = Nm$$

- from the Heisenberg equation of motion for the momentum operator we find

$$\frac{d^2 \hat{R}_\alpha}{dt^2} + \omega_\alpha^2 \hat{R}_\alpha = 0$$

The Kohn Theorem, cont'd

- this result is *independent* of the interactions between the particles. In other words, the centre-of-mass motion separates from the relative motion of the particles. This implies the existence of dipolar oscillations of the centre-of-mass at the frequencies ω_α .
- likewise, one can show that the nonlinear TDGP equation has a solution of the form

$$n_c(\mathbf{r}, t) = n_{c0}(\mathbf{r} - \boldsymbol{\eta}(t)), \quad \mathbf{v}_c(\mathbf{r}, t) = \dot{\boldsymbol{\eta}}(t)$$

where

$$\frac{d^2 \eta_\alpha(t)}{dt^2} = -\omega_\alpha^2 \eta_\alpha(t)$$

E: It is instructive to prove this.

- there is thus a solution where the condensate oscillates rigidly about the centre of the trap. A consequence of the Kohn theorem is that such a mode *must exist regardless of the state of relative motion of the atoms*. In fact, such a mode will exist even at finite temperature.