Advanced Quantum Mechanics

Rajdeep Sensarma

sensarma@theory.tifr.res.in

Lecture #15

Quantum Mechanics of Many Particles

Recap of Last Class

Writing Many Body Hamiltonians with creation annihilation operators

Ground State Energy -> Pressure, Compressibility

Free Fermi gas and its degeneracy pressure.

Free Bose Gas and BEC

Weakly Repulsive Bose gas

Consider a large number of bosonic particles (spin 0) interacting with each other by pair-wise contact interaction. The system has a homogeneous density ρ.

$$V(\vec{r}-\vec{r'}) = g\delta(\vec{r}-\vec{r'}) \qquad V(\vec{q}) = g$$

We will stick to 3D for the time being

$$H = \sum_k \frac{k^2}{2m} a_k^\dagger a_k + \frac{g}{2} \sum_{xx'} a_x^\dagger a_{x'}^\dagger a_{x'} a_x$$

$$H_I = \frac{1}{V} \sum_{k_1,k_2,k_3 k_4} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \sum_{x,x'} V(x-x') e^{i(k_1\cdot x + k_2 \cdot x' - k_3 \cdot x' - k_4 \cdot x)}$$

FT of the interaction term

$$H_I = \frac{g}{2V} \sum_{k_1,k_2,k_3 k_4} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \delta(k_1 + k_2 - k_3 - k_4)$$

$$H_I = \frac{g}{2V} \sum_{k,k',q} a_{k+q}^\dagger a_{k'-q}^\dagger a_{k'} a_k$$

So,

$$\boxed{H = \sum_k \frac{k^2}{2m} a_k^\dagger a_k + \frac{g}{2V} \sum_{k,k',q} a_{k+q}^\dagger a_{k'-q}^\dagger a_{k'} a_k}$$

ground state for non-interacting Bosons: $|\psi\rangle = \frac{\left(a_0^\dagger\right)^N}{\sqrt{N!}}|0\rangle$

How does this picture change in presence of interaction?

BEC in weakly repulsive Bose gas

For noninteracting system: $\langle a_0^\dagger a_0 \rangle = N_0 = N$ All Bosons are in the condensate

For weakly interacting system, still expect the occupation of the k=0 mode to be macroscopically large.

$$\langle a_0^\dagger a_0 \rangle = N_0 \simeq N$$ More precisely, $N_0/N \to \rho_0/\rho \neq 0$ as $N \to \infty$

Implicit defn. of weak interactions: 1- ρ_0/ρ << 1

In this limit, we can forget the fact that a_0 is an operator and replace it by its expectation value, a complex number, ϕ

with $$N_0 = |\phi|^2$$

This neglects fluctuations of the creation/annihilation operator (for k=0) which is ~ 1 compared to expectation values N_0~N.

$$[a_0, a_0^\dagger] = 1$$

Treating k=0 mode in classical approximation is OK.

This is like treating e-m radiation classically when we have large no. of photons.

Bogoliubov Theory of Weakly Repulsive BEC

Presence of interactions imply that even at T=0, not all Bosons are in k=0 mode

These finite k Bosons interact with themselves and with the condensate.

Bogoliubov Theory keeps interaction of Bosons with the condensate and throws out B-B interaction otherwise

Provides the leading Quantum Correction to the classical description of all particles in the Condensate.

Provides perturbation expansion in appropriate dimensionless coupling in weak coupling limit.

Bogoliubov Theory of Weakly Repulsive BEC

$$\hat{H} = \sum_k \frac{k^2}{2m} a_k^\dagger a_k + \frac{g}{2V} \sum_{kk'q} a_{k+q}^\dagger a_{k'-q}^\dagger a_{k'} a_k$$

Let us first separate out terms involving a_0

The K.E. contribution of the condensate term is 0 and we can focus on the interaction

$$\frac{g}{2V} \sum_{kk'q} a_{k+q}^\dagger a_{k'-q}^\dagger a_{k'} a_k = \frac{g}{2V} \Big[\; |\phi|^4 + \phi^2 \sum_k a_k^\dagger a_{-k}^\dagger + \phi^{*2} \sum_k a_{-k} a_k + 4|\phi|^2 \sum_k a_k^\dagger a_k +$$

All mom sums exclude 0

$$\cancel{2\phi \sum_{kq} a_q^\dagger a_{k-q}^\dagger a_k + 2\phi^* \sum_{kq} a_{k+q}^\dagger a_k a_q +}$$

Expansion in ϕ, Bogoliubov Theory

keeps the first leading correction ~ ϕ^2

$$\cancel{\sum_{kk'q} a_{k+q}^\dagger a_{k'-q}^\dagger a_{k'} a_k} \Big]$$

Leading Quantum Correction around Classical Theory

Bogoliubov Theory of Weakly Repulsive BEC

Assume real ϕ (will justify later)

$$\hat{H} = \sum_k \frac{k^2}{2m} a_k^\dagger a_k + \frac{g}{2V} \sum_{kk'q} a_{k+q}^\dagger a_{k'-q}^\dagger a_{k'} a_k$$

$$\frac{g}{2V} \sum_{kk'q} a_{k+q}^\dagger a_{k'-q}^\dagger a_{k'} a_k = \frac{g}{2V} \left[\; |\phi|^4 + \phi^2 \sum_k a_k^\dagger a_{-k}^\dagger + \phi^{*2} \sum_k a_{-k} a_k + 4|\phi|^2 \sum_k a_k^\dagger a_k \right]$$

All mom sums exclude 0

$$\phi^2 = N_0 = N - \sum_k a_k^\dagger a_k$$

Since we are interested in O(N) terms, it is OK to replace ϕ^2 by N in quadratic terms.

In ϕ^4 term corrections need to be taken into account $|\phi|^4 = N^2 - 2N \sum_k a_k^\dagger a_k + ..$

$$\hat{H} = \sum_k \left[\frac{k^2}{2m} + g\rho \right] a_k^\dagger a_k + \frac{g\rho}{2} \sum_k a_k^\dagger a_{-k}^\dagger + a_{-k} a_k$$

ρ is density of Bosons

Bogoliubov Theory of Weakly Repulsive BEC

$$\hat{H} = \sum_k \left[\frac{k^2}{2m} + g\rho\right] a_k^\dagger a_k + \frac{g\rho}{2}\sum_k a_k^\dagger a_{-k}^\dagger + a_{-k}a_k$$

Hamiltonian quadratic in creation/annihilation operators

Occupation basis of a is not eigenbasis of H

$$\hat{H} = -\frac{1}{2}\sum_k \frac{k^2}{2m} + g\rho + \frac{1}{2}\sum_k \begin{pmatrix} a_k^\dagger & a_{-k} \end{pmatrix} \begin{pmatrix} \frac{k^2}{2m} + g\rho & g\rho \\ g\rho & \frac{k^2}{2m} + g\rho \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix}$$

Occupation basis of linear combination of a_k and $a^\dagger_{-k}$ should be the eigenbasis of H

With linear transforms $\gamma_{\alpha k}^\dagger = u_k^\alpha a_k^\dagger + v_k^\alpha a_{-k}$ one should be able to write down

$$\hat{H} \sim E_0 + \sum_{\alpha k} E_k^\alpha \gamma_{\alpha k}^\dagger \gamma_{\alpha k}$$

Occupation number basis of γ would be eigenbasis

Bogoliubov Theory

Define new operators which are linear combinations of $a^\dagger_k$ and a_{-k}

$$\gamma_k^\dagger = u_k a_k^\dagger + v_k a_{-k} \qquad \gamma_{-k} = u_k a_{-k} + v_k a_k^\dagger$$

Used reflection symmetry
$u_k = u_{-k}$

Demand that new operators satisfy Bosonic commutation relations

$$[\gamma_k, \gamma_k^\dagger] = 1$$

$$= [u_k a_k + v_k a^\dagger_{-k}, u_k a_k^\dagger + v_k a_{-k}]$$

$$= |u_k|^2 \underbrace{[a_k, a_k^\dagger]}_{1} + |v_k|^2 \underbrace{[a^\dagger_{-k}, a_{-k}]}_{-1} + u_k v_k \underbrace{[a_k, a_{-k}]}_{0} + v_k u_k \underbrace{[a^\dagger_{-k}, a_k^\dagger]}_{0}$$

$$\boxed{|u_k|^2 - |v_k|^2 = 1}$$

$$\begin{pmatrix} \gamma_k^\dagger \\ \gamma_{-k} \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ v_k^* & u_k^* \end{pmatrix} \begin{pmatrix} a_k^\dagger \\ a_{-k} \end{pmatrix} \longrightarrow \begin{pmatrix} a_k^\dagger \\ a_{-k} \end{pmatrix} = \begin{pmatrix} u_k^* & -v_k^* \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} \gamma_k^\dagger \\ \gamma_{-k} \end{pmatrix}$$

Bogoliubov Theory

$$\begin{pmatrix} a_k^\dagger \\ a_{-k} \end{pmatrix} = \begin{pmatrix} u_k^* & -v_k^* \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} \gamma_k^\dagger \\ \gamma_{-k} \end{pmatrix}$$

$$a_k^\dagger a_k = |u_k|^2 \gamma_k^\dagger \gamma_k + |v_k|^2 \gamma_{-k}\gamma_{-k}^\dagger - (u_k^* v_k \gamma_k^\dagger \gamma_{-k}^\dagger + \ h.c.)$$

$$a_{-k} a_{-k}^\dagger = |v_k|^2 \gamma_k^\dagger \gamma_k + |u_k|^2 \gamma_{-k}\gamma_{-k}^\dagger - (u_k^* v_k \gamma_k^\dagger \gamma_{-k}^\dagger + \ h.c.)$$

$$a_k^\dagger a_{-k}^\dagger = -u_k^* v_k^* (\gamma_k^\dagger \gamma_k + \gamma_{-k}\gamma_{-k}^\dagger) + (u_k^*)^2 \gamma_k^\dagger \gamma_{-k}^\dagger + (v_k^*)^2 \gamma_{-k}\gamma_k .)$$

The Hamiltonian:

$$H = \frac{1}{2}\sum_k \left(\frac{k^2}{2m} + g\rho\right)(a_k^\dagger a_k + a_{-k}a_{-k}^\dagger) + g\rho(a_k^\dagger a_{-k}^\dagger + h.c.) \ -\frac{1}{2}\sum_k \left(\frac{k^2}{2m} + g\rho\right)$$

$$= \frac{1}{2}\sum_k \left\{ \left(\frac{k^2}{2m} + g\rho\right)(u_k^2 + v_k^2) - 2g\rho u_k v_k \right\} (\gamma_k^\dagger \gamma_k + \gamma_{-k}\gamma_{-k}^\dagger)$$

$$-\frac{1}{2}\sum_k \left\{ \left(\frac{k^2}{2m} + g\rho\right) 2u_k v_k + g\rho(u_k^2 + v_k^2) \right\} \gamma_k^\dagger \gamma_{-k}^\dagger \ + \ h.c. \ -\frac{1}{2}\sum_k \left(\frac{k^2}{2m} + g\rho\right)$$

If

=0

The Hamiltonian is diagonal in the number basis of γ operators

Bogoliubov Theory

Take $u_k = \cosh\theta_k \quad v_k = \sinh\theta_k$ Automatically satisfies $|u_k|^2 - |v_k|^2 = 1$

$u_k^2 + v_k^2 = \cosh 2\theta_k$ $2u_k v_k = \sinh 2\theta_k$

$$\left\{\left(\frac{k^2}{2m} + g\rho\right) 2u_k v_k - g\rho(u_k^2 + v_k^2)\right\} = 0 \longrightarrow \left\{\left(\frac{k^2}{2m} + g\rho\right) \sinh 2\theta_k - g\rho \cosh 2\theta_k\right\} = 0$$

$$\boxed{\tanh 2\theta_k = \frac{g\rho}{\frac{k^2}{2m} + g\rho}}$$

Define $$E_k = \sqrt{\left(\frac{k^2}{2m} + g\rho\right)^2 - g^2\rho^2}$$

$$u_k^2 = 1 + v_k^2 = \frac{1}{2}\left[1 + \frac{\frac{k^2}{2m} + g\rho}{E_k}\right] \qquad u_k v_k = \frac{g\rho}{2E_k}$$

Bogoliubov Theory

With these values of u_k and v_k

$$H = \frac{1}{2}\sum_k \left\{ \left(\frac{k^2}{2m} + g\rho\right)(u_k^2 + v_k^2) - 2g\rho u_k v_k \right\} (\gamma_k^\dagger \gamma_k + \gamma_{-k}\gamma_{-k}^\dagger) \; -\frac{1}{2}\sum_k \left(\frac{k^2}{2m} + g\rho\right)$$

Now, $$u_k^2 + v_k^2 = \frac{\frac{k^2}{2m} + g\rho}{E_k} \qquad u_k v_k = \frac{g\rho}{2E_k}$$

$$\left(\frac{k^2}{2m} + g\rho\right)(u_k^2 + v_k^2) - 2g\rho u_k v_k = \frac{\left(\frac{k^2}{2m} + g\rho\right)^2 - g^2\rho^2}{E_k} = E_k$$

$$H = \frac{1}{2}\sum_k E_k(\gamma_k^\dagger \gamma_k + \gamma_{-k}^\dagger \gamma_{-k}) + \frac{1}{2}\sum_k E_k - k^2/2m - g\rho$$

We have managed to obtain the eigenstates of the interacting Bose gas
(within Bogoliubov Approximation)

The Ground State

$$H = \frac{1}{2}\sum_k E_k(\gamma_k^\dagger \gamma_k + \gamma_{-k}^\dagger \gamma_{-k}) + \frac{1}{2}\sum_k E_k - k^2/2m - g\rho$$

Since E_k >= 0, the ground state corresponds to a state, where occ. no. of the γ Bosons is zero for all momentum states

$$\gamma_k|\psi_G\rangle = 0 \qquad \forall k$$

Ground state energy: $$U/V = \frac{1}{2}\sum_k E_k - k^2/2m - g\rho$$

We started Bogoliubov approximation by claiming $\rho_0 = \langle a_0^\dagger a_0\rangle \sim \rho$

Let us see when this approximation holds, i.e. when the above theory makes sense.

For this we will calculate $$\rho_0 = \rho - \sum_k \langle a_k^\dagger a_k\rangle$$

The Ground State

$$\rho_0 = \rho - \sum_k \langle a_k^\dagger a_k \rangle$$

$$\begin{pmatrix} a_k^\dagger \\ a_{-k} \end{pmatrix} = \begin{pmatrix} u_k^* & -v_k^* \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} \gamma_k^\dagger \\ \gamma_{-k} \end{pmatrix}$$

$$a_k^\dagger a_k = [u_k \gamma_k^\dagger - v_k \gamma_{-k}][u_k \gamma_k - v_k \gamma_{-k}^\dagger]$$

$$= u_k^2 \gamma_k^\dagger \gamma_k - u_k v_k (\gamma_k^\dagger \gamma_{-k}^\dagger + \gamma_{-k}\gamma_k) + v_k^2 \gamma_{-k}\gamma_{-k}^\dagger$$

Expectation value in GS: $\langle \psi_G | \gamma_k^\dagger \gamma_k | \psi_G \rangle = 0$

$$\langle \psi_G | \gamma_k^\dagger \gamma_{-k}^\dagger + \gamma_{-k}\gamma_k | \psi_G \rangle = 0$$

$$\langle \psi_G | \gamma_{-k}\gamma_{-k}^\dagger | \psi_G \rangle = \langle \psi_G | 1 + \gamma_{-k}^\dagger \gamma_{-k} | \psi_G \rangle = 1$$

No. of atoms in k ≠ 0 mode $\quad N' = \sum_k \langle a_k^\dagger a_k \rangle = \sum_k v_k^2 = \frac{1}{2} \sum_k \left(\frac{\frac{k^2}{2m} + g\rho}{E_k} - 1 \right)$

The Ground State

$$N' = \sum_k \langle a_k^\dagger a_k \rangle = \sum_k v_k^2 = \frac{1}{2}\sum_k \left(\frac{\frac{k^2}{2m} + g\rho}{E_k} - 1 \right)$$

$$N' = \frac{V}{(2\pi)^3}\frac{4\pi}{2}\int_0^\infty k^2 dk \left(\frac{\frac{k^2}{2m} + g\rho}{\sqrt{g\rho\frac{k^2}{m} + \left(\frac{k^2}{2m}\right)^2}} - 1 \right)$$

$$y = \frac{k}{\sqrt{2m\rho g}}$$

$$\rho' = \frac{1}{4\pi^2}(2m\rho g)^{3/2}\int_0^\infty y^2 dy \left(\frac{y^2+1}{\sqrt{2y^2+y^4}} - 1 \right) \longrightarrow \frac{\sqrt{2}}{3}$$

$$\frac{\rho'}{\rho} = \frac{\sqrt{2}}{12\pi^2\rho}(2m\rho g)^{3/2} = \frac{m^{3/2}}{3\pi^2}(\rho g^3)^{1/2} = \frac{8}{3\sqrt{\pi}}(\rho a_s^3)^{1/2}$$

scattering length

$$g = \frac{4\pi a_s}{m}$$

For Bogoliubov theory to be valid $\qquad \rho a_s^3 \ll 1$

Weakly Interacting / Dilute Bose gas