Lecture 6 : Bogoliubov theory of the dilute BEC

ground state of non-interacting Bose gas : $|N : \phi_0\rangle$,

ϕ_0 = ground state $\hat{h}_1$

$$\left[h_1 = -\frac{\hbar^2}{2m}\nabla^2 + V_{ext} = \text{1-particle hamilt} \right]$$

low-T, low excitation regime $\longrightarrow$ close to $|N : \phi_0\rangle$

ground state with weak interactions $\longrightarrow$ remains close to $|N : \phi_0\rangle$

$\hookrightarrow$ some BEC depletion to be expected by interactions

$\psi^\dagger \psi^\dagger \psi \psi$ term can destroy 2 BEC particles

and transfer them into excited states.

Bogoliubov theory is theory of lowest excitations in weakly interacting BECs

* based on systematic expansion in $\delta N / N$

* determines low-lying excited states in terms of

bosonic excitations (Landau framework of many-body)

* all quantum properties can be extracted from it

(BEC statistics, squeezing, Hawking radiation ...)

Basic idea : $\hat{\psi}(r) = \phi_0(r)\ \hat{a}_{\phi_0} + \delta\hat{\psi}(r)$

$\phi_0(r)$ → BEC wavef; $\hat{a}_{\phi_0}$ → BEC mode; $\delta\hat{\psi}(r)$ → non condensed field

$\rightarrow$ small parameter : $\delta\psi \sim \sqrt{\rho_{nc}}$, $\phi_0\,\hat{a}_0 \sim \sqrt{\rho_0} \gg \sqrt{\rho_{nc}}$

$\hookrightarrow$ $\varepsilon = \sqrt{\rho_{nc}/\rho_0} \ll 1$.

$\delta\hat{\psi}(r)$ = <u>transverse field</u>, orthogonal to $\phi_0(r)$

$$\delta\hat{\psi}(r) = Q\,\hat{\psi}(r)\,, \qquad Q = \mathbb{1} - |\phi_0\rangle\langle\phi_0|$$

orthogonal projector.

$$\int d^3r\; \phi_0^*(r)\,\delta\hat{\psi}(r) = 0$$

$$\left[\delta\hat{\psi}(r_1),\, \delta\hat{\psi}^\dagger(r_2)\right] = \delta(r_1 - r_2) - \phi_0(r_1)\,\phi_0^*(r_2)$$

Restrict to $\hat{N} = N$ subspace (<u>canonical ensemble</u>)

$$\underbrace{a^\dagger_{\phi_0} a_{\phi_0}}_{\hat{N}_{\phi_0}} + \underbrace{\int d^3r\; \delta\hat{\psi}^\dagger(r)\,\delta\hat{\psi}(r)}_{\delta\hat{N}} = N$$

$$\Longrightarrow \quad \hat{a}^\dagger_{\phi_0}\hat{a}_{\phi_0} = N - \delta\hat{N}$$

$$\Longrightarrow \quad \hat{a}^\dagger_{\phi_0}\hat{a}^\dagger_{\phi_0}\hat{a}_{\phi_0}\hat{a}_{\phi_0} = \hat{N}_{\phi_0}(\hat{N}_{\phi_0} - 1) =$$

$$= (N - \delta\hat{N})(N - \delta\hat{N} - 1) \simeq N(N-1) - 2N\,\delta\hat{N} + \ldots$$

<u>Rewrite</u> system Hamiltonian H in terms of $\delta\psi$ operators only:

* grand-canonical ensemble for transverse field particles
* BEC plays the role of reservoir.

$$H = \int d^3r \;\; \hat{\psi}^\dagger(r)\, h_1\, \hat{\psi}(r) \;+\; \frac{g}{2}\, \hat{\psi}^\dagger(r)\, \hat{\psi}^\dagger(r)\, \hat{\psi}(r)\, \hat{\psi}(r)$$

and replace $\hat{\psi}(r) = \phi_0(r)\, \hat{a}_{\phi_0} + \delta\hat{\psi}(r)$.

Keep terms up to $\delta\psi^2$ and neglect higher-order ones.

$\hookrightarrow$ up to this order $\longrightarrow$ no need of regularizing δ-potential.

$$H = \int d^3r \Big[\phi_0^* h_1 \phi_0 \; a^\dagger_{\phi_0} a_{\phi_0} + \left(\delta\psi^\dagger(r)\, h_1\, \phi_0(r)\; a_{\phi_0} + h.c \right) +$$
$$+ \delta\psi^\dagger h_1 \delta\psi \; +$$
$$+ \frac{g}{2} |\phi_0(r)|^2\; a^\dagger_{\phi_0} a^\dagger_{\phi_0} a_{\phi_0} a_{\phi_0} + g \left(\delta\psi^\dagger |\phi_0|^2 \phi_0 \cdot a^\dagger_{\phi_0} a_{\phi_0} a_{\phi_0} + h.c. \right)$$
$$+ \frac{g}{2} \left(\delta\hat{\psi}^\dagger(r)\, \delta\hat{\psi}^\dagger(r)\, \phi_0(r)^2 \cdot a^2_{\phi_0} + h.c. \right) +$$
$$+ 2g \left(\delta\psi^\dagger(r)\, \delta\psi(r)\; |\phi_0(r)|^2 \cdot a^\dagger_{\phi_0} a_{\phi_0} \right) \Big]$$

For simplicity: assume h_1 = time-independent

ϕ_0 = lowest μ solution of GPE at $\mu = \mu_0$

$$H = \int d^3r \left[\phi_0^* h_1 \phi_0 \;\hat{N}_{\phi_0} + \frac{g}{2} |\phi_0|^4 \;\hat{N}_{\phi_0} (\hat{N}_{\phi_0} - 1) \right] + \qquad (0)$$

$$+ \left\{ \delta\psi^\dagger(r) \left[h_1 \phi_0 + g |\phi_0|^2\; \hat{a}^\dagger_{\phi_0} \hat{a}_{\phi_0} \right] a_{\phi_0} + h.c. \right\} + \qquad (1)$$

$$\left.\begin{aligned} &+ \left\{ \delta\psi^\dagger h_1 \delta\psi + \frac{g}{2}\, \delta\psi^\dagger \delta\psi^\dagger\; \phi_0^2\; a^2_{\phi_0} + h.c \right\} + \\ &+ 2g |\phi_0|^2\; a^\dagger_{\phi_0} a_{\phi_0}\;\; \delta\psi^\dagger \delta\psi + \dots \end{aligned}\right\} \qquad (2)$$

$$H_0 = \int d^3r \; (\phi_0^* h_1 \phi_0) N + \frac{g}{2} |\phi_0|^4 N(N-1) \; +$$

$$- \left[\phi_0^* h_1 \phi_0 + g N |\phi_0|^2 \right] \delta\hat{N} = E_0(N) - \mu_0 \delta\hat{N}$$

$$H_1 = \int d^3r \; \delta\hat{\psi}^\dagger(r) \left[h_1 \phi_0 + g |\phi_0|^2 \hat{a}^\dagger_{\phi_0} \hat{a}_{\phi_0} \right] a_{\phi_0} + h.c.$$

$$\simeq \int d^3r \; \delta\hat{\psi}^\dagger(r) \left[h_1 \phi_0 + g N |\phi_0|^2 \right] \hat{a}_{\phi_0} + h.c. = 0$$

[correction $\sim \delta\hat{N} \; a_{\phi_0}$ is 3rd order]

$$H_2 = \int d^3r \; \delta\psi^\dagger h_1 \delta\psi + \left(\frac{g}{2} \phi_0^2 \delta\psi^\dagger \delta\psi^\dagger a^2_{\phi_0} + h.c. \right) +$$

$$+ 2g |\phi_0|^2 a^\dagger_{\phi_0} a_{\phi_0} \delta\psi^\dagger \delta\psi$$

$$H_{Bog} = E_0(N) + \int d^3r \; \delta\hat{\psi}^\dagger (h_1 - \mu_0) \delta\hat{\psi} \; +$$

$$+ \frac{g}{2} \left(\phi_0^2 \delta\psi^\dagger \delta\psi^\dagger a^2_{\phi_0} + h.c. \right) +$$

$$+ 2g |\phi_0|^2 a^\dagger_{\phi_0} a_{\phi_0} \delta\psi^\dagger \delta\psi$$

Introduce "quasi-particle" operators that transfer 1 particle from BEC $\longrightarrow$ transverse field modes

$$\left[\!\left[\quad \hat{\Lambda}^\dagger(r) = \frac{1}{\sqrt{N}} \delta\hat{\psi}^\dagger(r) \, \hat{a}_{\phi_0} \quad \right]\!\right]$$

* BEC = bath for $\delta\psi$ field
* $\Lambda(r)$ satisfy transverse Bose commutation:

$$[\Lambda, \Lambda] = 0, \quad [\Lambda(r_1), \Lambda^\dagger(r_2)] \simeq 1 - \phi_0(r_1) \phi_0^*(r_2)$$

* Λ conserve total $\hat{N}$

$$H_{Bog} = E_0(N) + \int d^3r \; \Lambda^\dagger(r)\,(h_1 - \mu_0)\,\Lambda(r) + $$
$$+ \frac{g}{2}\left(\phi_0^2\, \Lambda(r)\,\Lambda(r) + h.c.\right) +$$
$$+ 2g|\phi_0|^2\, \Lambda^\dagger(r)\,\Lambda(r) =$$

$$= E_0(N) + \frac{1}{2}\,(\Lambda^\dagger, \Lambda)\,\eta\,\mathcal{L}\begin{pmatrix}\Lambda \\ \Lambda^\dagger\end{pmatrix} \quad ; \quad \eta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

with $$\mathcal{L} = \begin{pmatrix} h_1 - \mu_0 + 2g|\phi_0|^2 & \frac{1}{2} g\,\phi_0^2 \\ -\frac{1}{2} g\,\phi_0^{*2} & -(h_1 - \mu_0 + 2g|\phi_0|^2) \end{pmatrix}$$

Heisenberg eqs. of motion:

$$i\hbar \frac{d}{dt}\begin{pmatrix}\Lambda \\ \Lambda^\dagger\end{pmatrix} = \begin{pmatrix} Q & 0 \\ 0 & Q^* \end{pmatrix}\mathcal{L}\begin{pmatrix}\Lambda \\ \Lambda^\dagger\end{pmatrix}$$

$\hookrightarrow$ preserves transversality of Λ,
comes from $[\Lambda, \Lambda^\dagger] \sim Q$

$$\mathcal{L}_\perp = \begin{pmatrix} Q & 0 \\ 0 & Q^* \end{pmatrix}\mathcal{L}$$

$\to$ from transverse to transverse space
$\to$ η - hermitian
$\to$ can be diagonalized into η-orthonormal eigenstates

$$(u_{n'}^*, v_{n'}^*)\,\eta\begin{pmatrix} u_n \\ v_n \end{pmatrix} = \delta_{n,n'}$$

$$\begin{pmatrix}\hat{\Lambda}(r) \\ \hat{\Lambda}^\dagger(r)\end{pmatrix} = \sum_n \begin{pmatrix} u_n(r) \\ v_n(r) \end{pmatrix}\hat{b}_n + \begin{pmatrix} v_n^*(r) \\ u_n^*(r) \end{pmatrix}\hat{b}_n^\dagger$$

$\hat{b}_n = \int d^3r \left(u_n^*(r)\,\hat{\Lambda}(r) - v_n^*(r)\,\hat{\Lambda}^\dagger(r)\right)$ are Bose operators:

$$[\hat{b}_n, \hat{b}_{n'}^\dagger] = \delta_{n,n'}, \quad [\hat{b}_n, \hat{b}_{n'}] = 0$$

In the b_n basis, H_{Bog} can be rewritten as collection of harmonic oscillators:

$$H_{Bog} = E_0(N) + \sum_n \hbar\omega_n \, \hat{b}_n^+ \hat{b}_n$$

$\omega_n \rightarrow$ eigenvalues of $\mathcal{L}_\perp$ corresponding to positive-norm eigenvectors

$$\int d^3 r \; |u_n|^2 - |v_n|^2 = +1$$

NOTES:

* this procedure possible only if all eigenvalues of $\mathcal{L}_\perp$ are real

* if ω_n is eigenvalue of $\mathcal{L}_\perp \Rightarrow \omega_n^*$ is also eigenvalue of $\mathcal{L}_\perp$

  $\hookrightarrow$ dynamical stability $\Rightarrow$ ω_n's are all real

* $\begin{pmatrix} u_n \\ v_n \end{pmatrix}$ eigenvector of $\mathcal{L}_\perp$ at ω_n

  $\Rightarrow \begin{pmatrix} v_n^* \\ u_n^* \end{pmatrix}$ is eigenvector at $-\omega_n$ with opposite η-norm

* if ϕ_0 is non-degenerate local minimum of $E_{GP}[\phi]$

  $\Rightarrow$ all ω_n's > 0

  Energetic (or thermodynamic) stability

Quantum and thermal condensate depletion

$$\hat{N}_0 = N - \int d^3r \; \delta\hat{\psi}^\dagger(r)\, \delta\hat{\psi}(r) \simeq N - \int d^3r \; \hat{\Lambda}^\dagger(r)\, \hat{\Lambda}(r)$$

$$\delta\hat{N} = \int d^3r \sum_{nn'} \left(v_n(r)\, \hat{b}_n + u_n^*(r)\, \hat{b}_n^\dagger\right) \left(u_{n'}(r)\, \hat{b}_{n'} + v_{n'}^*(r)\, \hat{b}_{n'}^\dagger\right)$$

Thermal equil. state : $\langle b_n b_{n'} \rangle = 0$

$$\langle b_n^\dagger b_{n'} \rangle = \delta_{n,n'} \frac{1}{e^{\beta\hbar\omega_n} - 1}$$

$$\langle \delta\hat{N} \rangle = \int d^3r \sum_k |v_n(r)|^2 \langle \hat{b}_n \hat{b}_n^\dagger \rangle + |u_n(r)|^2 \langle b_n^\dagger b_n \rangle$$

homogeneous system : $u_n(r) = \frac{1}{\sqrt{V}}\, u_n\, e^{ikr}$

$$v_n(r) = \frac{1}{\sqrt{V}}\, v_n\, e^{ikr}$$

with $u_n + v_n = \left(\frac{\hbar^2 k^2/2m}{\omega_n}\right)^{1/2}$

$$u_n - v_n = \left(\frac{\omega_n}{\hbar^2 k^2/2m}\right)^{1/2}$$

$$\langle \delta\hat{N} \rangle = \int \frac{V}{(2\pi)^3}\, d^3k \left[\left(|u_n|^2 + |v_n|^2\right) \frac{1}{e^{\beta\hbar\omega_n} - 1} + |v_n|^2\right] =$$

$$= \langle \delta\hat{N} \rangle_{T=0} + \langle \delta\hat{N} \rangle_T .$$

$$\langle \delta\hat{N}\rangle_{T=0} = \int \frac{V}{(2\pi)^3}\, d^3k \cdot \left[\frac{1}{2}\left(\left(\frac{E_k}{\omega_k}\right)^{1/2} - \left(\frac{\omega_k}{E_k}\right)^{1/2}\right)\right]^2 =$$

$$= \int \frac{V}{(2\pi)^3}\, \frac{d^3k}{4}\, \frac{(E_k - \omega_k)^2}{\omega_k E_k} =$$

$$= \int \frac{V}{(2\pi)^3}\, \frac{d^3k}{4} \left(\frac{E_k^2 + \omega_k^2}{\omega_k E_k} - 2\right) =$$

$$= \int \frac{V}{(2\pi)^3}\, \frac{d^3k}{4} \left(\frac{E_k^2 + E_k^2 + 2\mu E_k}{\omega_k E_k} - 2\right)$$

$$= \int \frac{V}{(2\pi)^3}\, \frac{d^3k}{2} \left(\frac{E_k + \mu}{\omega_k} - 1\right)$$

$$\frac{E_k}{2\mu} = \frac{\hbar^2 k^2}{4m\mu} = q^2$$

$$\frac{\omega_k}{2\mu} = \frac{\sqrt{E_k(E_k + 2\mu)}}{2\mu} = q\,(q^2+1)^{1/2}$$

$$d^3k = 4\pi k^2\, dk = 4\pi \left(\frac{4m\mu}{\hbar^2}\right)^{3/2} q^2\, dq$$

$$= \frac{V}{(2\pi)^3} \cdot 2\pi \left(\frac{4mg\rho}{\hbar^2}\right)^{3/2} \cdot \int_0^\infty dq\; q^2 \left(\frac{q^2 + 1/2}{q\,(q^2+1)^{1/2}} - 1\right)$$

$$\frac{\langle \delta N\rangle_{T=0}}{N} = \frac{1}{(2\pi)^2 \rho} \left(\frac{4\cancel{m}\, \frac{4\pi\hbar^2 a}{\cancel{m}}\, \rho}{\cancel{\hbar^2}}\right)^{3/2} \quad \#$$

$$= (a^3\rho)^{1/2}\, \frac{(16\pi)^{3/2}}{4\pi^2}\, \# = (\rho a^3)^{1/2}\, \frac{16}{\sqrt{\pi}}\, \# = \frac{8}{3\sqrt{\pi}}\, (\rho a^3)^{1/2}$$

[$\longrightarrow$ diluteness of the gas $\sim \underline{(\rho a^3)^{1/2}}$ parameter]

Bogoliubov approach is consistent if $(\rho a^3)^{1/2} \ll 1$

$\rightarrow$ ok for ultracold atoms

$\rightarrow$ fails for liquid ^4He

NOTE: Bogoliubov excitations $\neq$ non-condensed particles.

Thermal depletion

$$\frac{\langle \delta \hat{N} \rangle_T}{N} = \frac{32}{\sqrt{\pi}} \int_0^{\infty} dq \, \frac{q(q^2+1/2)}{(q^2+1)^{1/2}} \exp\left[\left(2\beta g\rho \, q(q^2+1)^{1/2}\right)-1\right]^{-1}$$

* low-temperature limit $T \ll \mu$:

$$\frac{\langle \delta N \rangle_T}{N} = \frac{\langle \delta N \rangle_0}{N} \cdot \left(\frac{\pi k_B T}{2\mu}\right)^2 + \dots$$

* high-temperature limit $T \gg \mu$:

$$\frac{\langle \delta N \rangle_T}{N} \simeq \frac{\zeta(3/2)}{\rho \lambda_{dB}^3}$$ as expected from non-interacting gas.

$\rightarrow$ holds only for $\langle \delta N \rangle_T \ll T$

$\rightarrow$ Result is consistent as $\rho \lambda_{dB}^3 (T=\mu) \gg 1$:

$$\lambda_{dB} = \left(\frac{2\pi\hbar^2}{m k_B T}\right)^{1/2} \qquad \rho \lambda_{dB}^3 (T=\mu) = \rho \left(\frac{2\pi\hbar^2}{m g\rho}\right)^{3/2} =$$

$$= \left(\frac{2\pi\hbar^2}{m \cdot \frac{4\pi\hbar^2 a}{m}\rho}\right)^{3/2} \cdot \rho = \frac{\rho}{(2a\rho)^{3/2}} = \frac{1}{(2a\rho^{1/3})^{3/2}} = \frac{1}{\sqrt{8(\rho a^3)}} \gg 1$$

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→ discussion of regularization issues for the Dirac-δ potential