Lect 5. mean field theory of Superfluid

§1. Review of second quantization

$\psi(r) \longrightarrow$ field operator $\hat{\psi}(r) = \sum_k \frac{1}{\sqrt{V}} e^{ikr} \hat{a}_k$.

$\rho(r) = \psi^*(r)\psi(r) \quad \rightarrow \quad \rho(r) = \hat{\psi}^+(r)\psi(r)$

$H_0 = \sum_i \frac{-\hbar^2}{2m} \nabla_i^2 \quad \rightarrow \quad H_0 = \int dr\, \hat{\psi}^+(r) \left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi(r)$

$= \sum_k a_k^+ a_k \varepsilon_k$

$H_{int} = \frac{1}{2}\int dr\, dr'\, \psi^+(r)\psi^+(r')\psi(r')\psi(r) \quad \rightarrow \quad H_{int} = \frac{1}{2}\int dr\, dr'\, \hat{\psi}^+(r)\hat{\psi}^+(r')\hat{\psi}(r')\psi(r)$

$= \frac{1}{2V}\sum_{q,P_1P_2} V(q)\, a^+_{P_1+q} a^+_{P_2-q} a_{P_2} a_{P_1}$

§2. Bosonic system

$$H = \int dr\, \psi^+(r)\Big(\underbrace{-\frac{\hbar^2}{2m}\nabla^2}_{-\mu}\Big)\psi(r) + \int dr\, dr'\, \frac{1}{2}\rho(r) V(r-r')\rho(r')$$

$$= \sum_k (\varepsilon_k - \mu)\, a_k^+ a_k + \frac{1}{2V}\sum_{kk'q} V_q\, a^+_{k'-q} a^+_{k+q} a_k a_{k'}$$

where $V_q = \int dr\, V(r)\, e^{ikr}$

we assume that, there's a macroscopic number of particles occupying $k=0$ state. i.e. $\langle\Omega|a_0^\dagger a_0|\Omega\rangle = N_0 \sim O(N)$. Then we can neglect the commutation relation $[a_0, a_0^\dagger]=1 \rightarrow [\frac{a_0}{\sqrt{N_0}}, \frac{a_0^\dagger}{\sqrt{N_0}}] = \frac{1}{N_0} \rightarrow 0.$

$$H_{mean} = \sum_k (\mathcal{E}_k - \mu) a_k^\dagger a_k + \frac{V}{2} \rho_0^2 V_0 + \frac{\rho_0}{2} \sum_{k\neq 0} (2 a_k^\dagger a_k V_0$$

$$+ 2a_k^\dagger a_k V_k + V_k a_{-k} a_k + V_k a_{-k}^\dagger a_k^\dagger)$$

$$= \sum_k (\mathcal{E}_k - \mu_k') a_k^\dagger a_k + \frac{1}{2}\rho_0^2 V_0 \cdot V + \frac{\rho_0}{2}\sum_{k\neq 0} V_k (a_{-k} a_k + a_{-k}^\dagger a_k)$$

$\mu_k' = \mu - \rho_0 V_0 - \rho_0 V_k$, $\rho_0 = N_0/V$. we have neglected term at $(a_{k\neq 0})^3$.

$$H_{mean} = \sum_k{}' (a_k^\dagger \;\; a_{-k}) \begin{pmatrix} \mathcal{E}_k - \mu_k' & \rho_0 V_k \\ \rho_0 V_k & +(\mathcal{E}_k - \mu_k') \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix}$$

$$- \frac{1}{2} \sum_k{}' (\mathcal{E}_k - \mu_k') + \frac{V}{2} \rho_0^2 V_0$$

define Bogoliubov transformation $\begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix}$

It's easy to check α_k, satisfies the commutator relation

$[\alpha_k, \alpha_{k'}^{+}] = \delta_{kk'}$, we need to determine the value of angle of θ_k to diagonalize the matrix.

$$\begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} \varepsilon_k - \mu_k' & \rho_0 V_k \\ \rho_0 k & \varepsilon_k - \mu_k' \end{pmatrix} \begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cos\theta_k \end{pmatrix}$$

$$= \begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} (\varepsilon_k - \mu_k')\cosh\theta_k + \rho_0 V_k \sinh\theta_k, & (\varepsilon_k - \mu_k')\sinh\theta_k + \rho_0 V_k \cos\theta_k \\ \rho_0 k \cosh\theta_k + (\varepsilon_k - \mu_k')\sinh\theta_k, & \rho_0 k \sinh\theta_k + (\varepsilon_k - \mu_k')\cos\theta_k \end{pmatrix}$$

$$= \begin{pmatrix} (\varepsilon_k - \mu')\cos 2\theta_k + \rho_0 V_k \sin 2\theta_k, & \rho_0 V_k \cos 2\theta_k + (\varepsilon_k - \mu_k')\sin 2\theta_k \\ \rho_0 V_k \cos 2\theta_k + (\varepsilon_k - \mu')\sin 2\theta_k, & (\varepsilon_k - \mu')\cos 2\theta_k + \rho_0 V_k \sin 2\theta_k \end{pmatrix}$$

we set $\rho_0 V_k \cos 2\theta_k + (\varepsilon_k - \mu_k')\sin 2\theta_k = 0 \Rightarrow \tanh 2\theta_k = -\dfrac{\rho_0 V_k}{\varepsilon_k - \mu_k'}$,

$$\cosh 2\theta = \frac{\varepsilon_k - \mu_k'}{\sqrt{(\varepsilon_k - \mu_k)^2 - (\rho_0 V_k)^2}}$$

$$\sinh 2\theta = \frac{-\rho_0 V_k}{\sqrt{(\varepsilon_k - \mu_k)^2 - (\rho V_k)^2}}$$

$\Rightarrow$

$$H_{mean} = \sum_k{}' (\alpha_k^{+} \ \alpha_{-k}) \begin{pmatrix} E_k & 0 \\ 0 & E_k \end{pmatrix} \begin{pmatrix} \alpha_k \\ \alpha_{-k}^{+} \end{pmatrix}$$

$$- \frac{1}{2}\sum_k{}' (\varepsilon_k - \mu_k') + \frac{V}{2}\rho_0^2 V_0$$

where $E_k = \sqrt{(\varepsilon_k - \mu_k)^2 - (\rho_0 V_k)^2}$, $\quad H_{mean} = \sum_{k \neq 0} E_k \alpha_k^{+} \alpha_k + \underline{V(-\mu\rho_0 + \frac{1}{2}\rho_0^2 V_0)} - \sum_{k \neq 0} \frac{1}{2}(\varepsilon_k - \mu_k' - E_k)$

contribution at $k=0$

The value of μ is set by minimizing Ω_g, respect to N_0.

$$\partial \Omega_g / \partial N_0 = 0 \qquad \Omega_g = V\left(-\mu \rho_0 + \tfrac{1}{2}\rho_0^2 V_0\right) \Rightarrow \boxed{\rho_0 = \frac{\mu}{V_0}}$$

keep terms at linear order of V_k

$$N = \langle \Omega | \sum_k a_k^+ a_k | \Omega \rangle = N_0(\mu) + \sum_k (\sinh \theta_k)^2 .$$

$$= V\left[\rho_0(\mu) + \int \frac{d^d k}{(2\pi)^d} \sinh^2 \theta_k\right] \Rightarrow$$

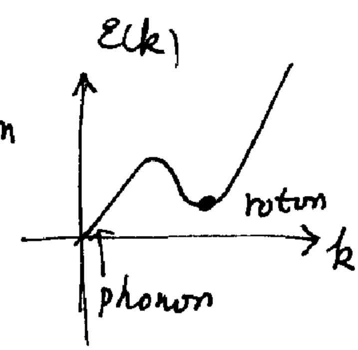
$$\boxed{\rho = \frac{\mu}{V_0} + \int \frac{d^d k}{(2\pi)^d} \sinh^2 \theta_k}$$

$$\Rightarrow E_k^2 = (\varepsilon_k + \rho_0 V_k)^2 - (\rho_0 V_k)^2 \Rightarrow E_k = \sqrt{\varepsilon_k(\varepsilon_k + 2\rho_0 V_k)}$$

at small $k \Rightarrow$ $E_k = v|k|$ with $v = \sqrt{\dfrac{\rho_0 V_0}{m}}$

The linear dispersion at $k=0$ in the above calculation is the result of $\rho_0 V(k=0) = \mu$, which is a mean-field result. The linear dispersion relation even holds at aritrary order of interaction strength.

The actural spectrum is Helium-4: phonon & Roton



§ Ground state properties of ^4He

The many-body ground state wavefunction $\varphi(R_1 \cdots R_n)$ is positive definite

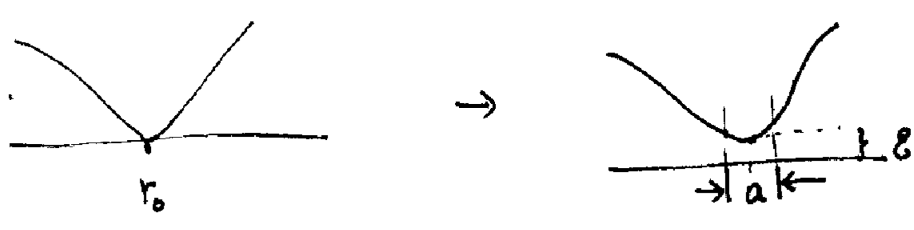
$\varphi(R_1 \cdots R_n)$ satisfies $\left[-\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} V(r_{ij})\right]\varphi = E\varphi$, and symmetry constraint.

$$\langle E\rangle = \frac{\int \varphi H \varphi \, d^N R}{\int \varphi \varphi \, d^N R} = \frac{\int \frac{1}{2m}\sum_i (\nabla_i \varphi)^2 + \sum V \varphi^2}{\int \varphi^2 \, d^N R}.$$

If φ has nodes,  , we can try $|\varphi(r_1, \cdots r_N)|$,

which will give the same $|\nabla_i \varphi|^2$ and $|\varphi_i|^2$, and thus $\langle E\rangle$.

However, we can soften the kink a litte bit, $\nabla\varphi$ changes from $|\nabla\varphi|_{r_0} \to 0$



$$\to \frac{\Delta E}{Vol} = - |\nabla\varphi|^2_{r_0 \to 0} \frac{1}{2m} + (|\nabla\varphi|_{r_0} \cdot a)^2 \cdot V$$

as "a" goes small,

we can gain energy by making

$\varphi(r_1 \cdots r_n)$ positive definite.

This also showes that Ground state is no degenerate. Because any two positive-definit wavefunction cannot be orthogonal to each other.

§ Single mode approximation

Excition $|\psi_k\rangle = \rho_k |\Phi_0\rangle$, where $\rho_k = \sum_{j=1}^{N} e^{i\vec{k}\cdot\vec{r}_i}$

$$\Rightarrow E_k - E_0 = \frac{\langle \psi_k | H - E_0 | \psi_k\rangle}{\langle \psi_k | \psi_k \rangle} = \frac{\langle \Phi_0 | \rho_{-k} (H - E_0) \rho_k | \Phi_0\rangle}{\langle \Phi_0 | \rho_{-k} \rho_k | \Phi_0 \rangle}$$

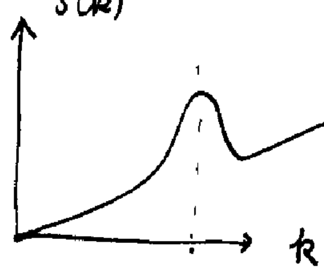
$$\langle \Phi_0 | \rho_{-k} (H - E_0) \rho_k | \Phi_0 \rangle = \langle \Phi_0 | \rho_{-k} [H - E_0, \rho_k] | \Phi_0 \rangle = \frac{1}{2} \langle \Phi_0 | [\rho_{-k}, [H - E_0, \rho_k]] | \Phi_0 \rangle$$

$$[\rho_{-k}, [H - E_0, \rho_k]] = \frac{\hbar^2 k^2}{2m}$$

$$\Rightarrow E_k - E_0 = \frac{\hbar^2 k^2}{2m} \frac{1}{S(k)}, \quad \text{where } S(k) = \int dk\, e^{i\vec{k}(\vec{r}-\vec{r}')} \langle \Phi_0 | \rho(r) \rho(r') | \Phi_0 \rangle$$

$$= \langle \Phi_0 | \rho_{-k} \rho_k | \Phi_0 \rangle$$

The neutron scattering shows



at $k \to 0$, $S(k)$ is linear $\sim \xi k$ with k, $\Rightarrow E_k - E_0 = \frac{\hbar^2}{2m\xi} k$,

$S(k)$ develops a hump at $k \sim 1/a$, $\to$ roton minimum.