3 Second Quantized Models

3.1 Free electron gas

For a system of non-interacting N-electrons, we have

$$H_0 = \sum_{n=1}^{N} \frac{p_n^2}{2m} \to H_0 \psi_0^N = E_0^N \psi_0^N \tag{3.1}$$

$$\psi_0^N = \frac{1}{\sqrt{N!}} \sum_p (-)^P \varphi_{\sigma_1}(r_{P1} ... \varphi_{\sigma_N}(r_{PN}), \tag{3.2}$$

$$\text{with } \int d^3 r \varphi_\sigma^*(r) \varphi_{\sigma'}(r) = \delta_{\sigma\sigma'} \to \varphi(r)_\sigma = \frac{1}{\sqrt{V}} \sum_k c_{k,\sigma} e^{ik\cdot r} \tag{3.3}$$

$$\begin{aligned} E_0^N = \sum_{n=1}^{N} \epsilon_n \to \epsilon &= \sum_{\sigma,\sigma'} \int d^3 r \varphi_\sigma^*(r) \frac{p^2}{2m} \varphi_{\sigma'}(r) \\ &= \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma},\ \epsilon_k = \frac{\hbar^2 k^2}{2m} \end{aligned} \tag{3.4}$$

Second quantization

$$\epsilon \to \hat{H} = \sum_{k,\sigma} \epsilon_k \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\sigma},\ \{\hat{c}_{k,\sigma}, \hat{c}_{k',\sigma'}^\dagger\} = \delta_{kk'} \delta_{\sigma\sigma'} \tag{3.5}$$

Fermi surface: Fermi momentum and Fermi energy

$$\sum_\sigma \langle c_{k,\sigma}^\dagger c_{k,\sigma} \rangle = 2n_k,\ n_k = 0, 1 \tag{3.6}$$

Assume a standing wave in a cubic volume $V = L^3$, we will have

$$\psi_{n_x,n_y,n_z}(x,y,z) = \frac{1}{\sqrt{V}} \sin(k_x x) \sin(k_y y) \sin(k_z z) \tag{3.7}$$

$$k = (k_x, k_y, k_z),\ k_x = \frac{\pi n_x}{L},\ k_y = \frac{\pi n_y}{L},\ k_z = \frac{\pi n_z}{L} \tag{3.8}$$

$$k^2 = k_x^2 + k_y^2 + k_z^2 = \frac{\pi^2}{L^2}(n_x^2 + n_y^2 + n_z^2) = \frac{\pi^2}{L^2} n^2 \tag{3.9}$$

$$\epsilon_k = \frac{\pi^2 \hbar^2}{2mL^2} n^2 \tag{3.10}$$

with $n = (n_x, n_y, n_z)$ where $n_x, n_y, n_z = 1, 2, 3, ...,$ and $n^2 = n_x^2 + n_y^2 + n_z^2$. From (9) we can see that $|n| = \frac{L}{\pi}|k|$. Let n is number of occupied states, $n_k = 1$, then we have

$$N = \int dV_n = 2 \times \frac{1}{8} \times \frac{L^3}{\pi^3} \int d^3k \tag{3.11}$$

$$= 2 \times \frac{V}{(2\pi)^3} 4\pi \int_0^{k_F} k^2 dk = 2 \times \frac{V}{(2\pi)^3} \frac{4\pi}{3} k_F^3 \tag{3.12}$$

$$\rightarrow k_F = \left(3\pi^2 n_V\right)^{1/3}, \quad n_V = \frac{N}{V} \tag{3.13}$$

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2 (3\pi^2 n_V)^{2/3}}{2m} \tag{3.14}$$

Note that a factor $2 = 2s + 1$, where s is the spin of fermion, i.e. electron spin is $s = \frac{1}{2}$, and a factor $\frac{1}{8}$ comes from a chosen quadrant of positive integers in 3D number space $\vec{n} = (n_x, n_y, n_z)$.

Density of state, with $E = \frac{\hbar^2 k^2}{2m} \rightarrow k^2 = \frac{2mE}{\hbar^2}$, we have

$$(13) \rightarrow N = \frac{V}{3\pi^2} k^3 = \frac{V}{3\pi^2} \left(\frac{2mE}{\hbar^2}\right)^{3/2} \equiv N(E) \tag{3.15}$$

$$D(E) = \frac{dN(E)}{dE} = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} \tag{3.16}$$

$$\rightarrow D(E) \propto E^{1/2} \tag{3.17}$$

The number of occupied states per unit energy E grows up as $E^{1/2}$.

System at finite temperature T, with $\beta = 1/k_B T$, we have particle distribution at energy ϵ in the form

$$n(\epsilon) = \frac{1}{e^{\beta(\epsilon - \mu)} + 1} = \frac{1}{z^{-1} e^{\beta\epsilon} + 1}, \; \mu = E_F \text{ and } z = e^{\beta\mu} \tag{3.18}$$

where $\epsilon - \mu > 0$ is for particle, while $\epsilon - \mu < 0$ is for hole, in the particle-hole picture, see Figure (3.1). Fermi temperature T_F is determined from the Fermi energy E_F as

$$E_F = k_B T_F \rightarrow T_F = \frac{E_F}{k_B} \tag{3.19}$$

For typical system with $E_F = 2eV \rightarrow T_F = 2 \times 10^4 K$.

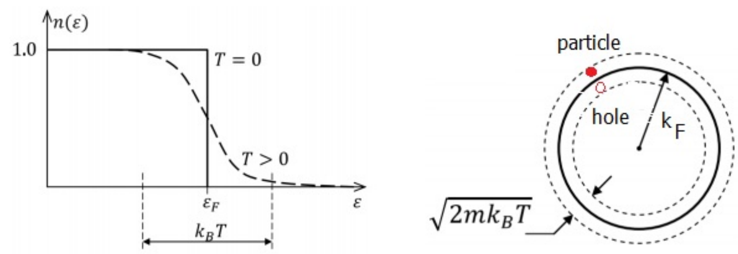

Figure 3.1:

3.2 Free Bose gas

For a system of non-interacting N-bosons, we have

$$H_0 = \sum_n \frac{p_n^2}{2m} \to H_0\psi_0^N = E_0^N\psi_0^N \to E_0^N = \langle\psi_0^N|H_0|\psi_0^N\rangle \tag{3.20}$$

$$\psi_0^N = \frac{1}{\sqrt{N!}}\sum_P (+)^P \varphi_{\alpha_1}(r_{P1})...\varphi_{\alpha_N}(r_{PN}) \tag{3.21}$$

$$\varphi(r) = \frac{1}{\sqrt{V}}\sum_q b_q e^{iq\cdot r} \tag{3.22}$$

In one-particle approximation

$$E_0^N = \sum_{n=1}^N \epsilon_n \to \epsilon = \int d^3r\varphi^*(r)\frac{p^2}{2m}\varphi(r) = \sum_q \epsilon_q b_q^\dagger b_q,\ \epsilon_q = \frac{\hbar^2q^2}{2m} \tag{3.23}$$

Second quantization

$$\epsilon \to H = \sum_q \epsilon_q b_q^\dagger b_q,\ [b_q, b_{q'}^\dagger] = \delta_{qq'} \tag{3.24}$$

Actually at zero temperature $T = 0K$, all bosons will occupy in their ground state at energy $\epsilon_0 = 0$. This is called *Bose-Einstein Condensation* or BEC. Anyway, to get some information of the system let us determine it at some finite temperature T, the particle distribution at energy ϵ is

$$n(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)} - 1} \tag{3.25}$$

We can determine the number of particles occupied in their ground state as

$$n(\epsilon_0) = \frac{1}{e^{-\beta\mu} - 1} \sim \frac{1}{1 - \beta\mu + ... - 1} \sim -\frac{1}{\beta\mu},\ \text{with } \epsilon_0 = 0 \tag{3.26}$$

This number diverges at $\mu \to 0$. We may set a macroscopic number N_0, as the onset of BEC, then we have

$$N_0 = \frac{1}{\beta|\mu|} \to |\mu| = \frac{k_B T}{N_0} \to z = e^{\beta\mu} \sim 1 + \beta\mu = 1 - \beta|\mu| \tag{3.27}$$

$$\to 1 - z = \frac{1}{N_0} \tag{3.28}$$

Next let us evaluate the total number distribution $n = N/V$ is

$$n = \int_0^\infty \frac{D(\epsilon)d\epsilon}{e^{\beta(\epsilon-\mu)} - 1} + \frac{2s+1}{V}\frac{z}{1-z} \tag{3.29}$$

$$D(\epsilon) = A\sqrt{\epsilon},\ A = \frac{2s+1}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \tag{3.30}$$

Since

$$\lim_{\mu\to 0}\int_0^\infty \frac{A\sqrt{\epsilon}d\epsilon}{e^{\beta(\epsilon-\mu} - 1} = \frac{A}{\beta^{3/2}}\int_0^\infty \frac{\sqrt{x}dx}{e^x - 1} = \frac{A}{\beta^{3/2}} \cdot 2.61$$

Then we have

$$n = 2.61A(k_B T)^{3/2} + \frac{2s+1}{V}\frac{1}{e^{-\beta\mu} - 1} \tag{3.31}$$

There is a critical temperature T_c such that

$$n = 2.61A(k_B T_c)^{3/2} = 2.61\frac{2}{\sqrt{\pi}}\frac{2s+1}{\lambda_c^3},\ \text{with } \lambda_c = \sqrt{\frac{h^2}{2\pi m k_B T_c}} \tag{3.32}$$

where λ_c is called *thermal wavelength*. Note that the BEC transition takes place at

$$\frac{n\lambda_c^3}{2s+1} = 2.62 \times \frac{2}{\sqrt{\pi}} \simeq 2.9$$

when λ_c is about inter-particle distance.

3.3 Phonons

For a crystalline system with lattice vector $\vec{R} = n_1\hat{a}_1 + n_2\hat{a}_2 + n_3\hat{a}_3$, within Born-Oppenheimer approximation the lattice Hamiltonian will be

$$H = \sum_{i=1}^{N}\frac{P_i^2}{2M} + V(R_1, R_2, ..., R_N) \tag{3.33}$$

Let R_0 is the equilibrium lattice position, i.e., minimum energy, let us do the Taylor's expansion of the potential with small fluctuation $R = R_0 + u$, we will have

$$V(\{R\}) = V(\{R_0\}) + \underbrace{\sum_i u_i V_i(\{R_0\})}_{=0} + \frac{1}{2}\sum_{i,j} u_i u_j V_{ij}(\{R_0\}) \tag{3.34}$$

Let us set $V(\{R_0\}) = 0$ for simplicity, and define $K_{ij} = V_{ij}(\{R_)\})$, small lattice oscillations Hamiltonian will be

$$H = \sum_i \frac{\pi_i^2}{2M} + \frac{1}{2}\sum_{ij} u_i u_j K_{ij},\ \pi_i = M\dot{u}_i \tag{3.35}$$

This appear with system of classical harmonic oscillators. After its first and second quantization we will have

$$H = \sum_{q,\alpha} \hbar\omega_{k,\alpha}(b^\dagger_{q,\alpha} b_{q,\alpha} + \frac{1}{2}),\ \omega_\alpha^2 = \frac{K_\alpha}{M} \tag{3.36}$$

where $\alpha = 1, 2$ for longitudinal (acoustic) and transverse (optical) branches, respectively.

3.4 Magnons

Magnetic matter is describe with Heisenberg's Hamiltonian

$$H = -J \sum_{<ij>} S_i \cdot S_j \tag{3.37}$$

where J is magnetic coupling constant, i.e., $J > 0$ for ferromagnet and $J < 0$ for anti-ferromagnet, and $< ij >$ is nearest neighbor sites. Note that $S = (S_x, S_y, S_z)$ is spin operator. We also use raising and lowering spin operators of the form $S^\pm = S_x \pm iS_y$.

Apply Holstein-Primakoff transformation

$$S^+ = \sqrt{1 - b^\dagger b}b,\ S^- = b^\dagger\sqrt{1 - b^\dagger b},\ S_z = \frac{1}{2} - b^\dagger b \tag{3.38}$$

Then we have

$$\begin{aligned} S_i \cdot S_j &= S_{ix}S_{jx} + S_{iy}S_{jy} + S_{iz}S_{jz} \\ &= \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) + S_{iz}S_{jz} \qquad (3.39) \\ &= \frac{1}{2}\left(b_i b_j^\dagger + b_i^\dagger b_j - b_i^\dagger b_i - b_j^\dagger b_j + \frac{1}{2}\right) + O(b^4) \qquad (3.40) \end{aligned}$$

Since all spin align in some particular direction when temperature is below Curie temperature T_C. So that we assume $b_i^\dagger b_i = 1$ at $T < T_C$, from (3.37) we have

$$H = \underbrace{-\frac{3J}{4}N(N-1)}_{=E_0} - \frac{J}{2}\sum_{<ij>}(b_i^\dagger b_j + b_i b_j^\dagger) \tag{3.41}$$

Apply the plane wave expansion

$$b_i = \frac{1}{N^{3/2}}\sum_k b_k e^{ik\cdot x_i},\ b_k = \frac{1}{N^{3/2}}\sum_i b_i e^{-ik\cdot x_i} \tag{3.42}$$

$$b_j = b_{i+1} = \frac{1}{N^{3/2}}\sum_k b_k e^{ik\cdot(x_i+a)} \tag{3.43}$$

Then we have

$$H = E_0 + \sum_k \omega_k b_k^\dagger b_k,\ \omega_k = \frac{|J|}{2}(2-\cos(k\cdot a)) \tag{3.44}$$

There is *magnon* excitation spectrum over the magnetic ground state.