2 Theoretical Methods

2.1 Quantum oscillators

Classical harmonic oscillation is a system of simple oscillation, its Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2,\ \omega^2 = \frac{k}{m} \tag{1}$$

Its quantization is

$$x \to \hat{x} = x,\ p \to \hat{p} = -i\hbar\frac{d}{dx},\quad [\hat{x},\hat{p}] = i\hbar \tag{2}$$

$$H \to \hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2,\ \hat{H}|\psi_E\rangle = E|\psi_E\rangle \tag{3}$$

2.1.1 Bose oscillator

Let us define

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a}),\ \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^\dagger - \hat{a}) \tag{4}$$

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{i}{m\omega}\hat{p}),\ \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{i}{m\omega}\hat{p}) \tag{5}$$

$$[\hat{a},\hat{a}] = 0 = [\hat{a}^\dagger,\hat{a}^\dagger],\ [\hat{a},\hat{a}^\dagger] = 1 \tag{6}$$

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}) \tag{7}$$

We just looking for

$$\hat{N} = \hat{a}^\dagger\hat{a} \xrightarrow{?} \hat{N}|n\rangle = n|n\rangle \tag{8}$$

$$\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2}),\ [\hat{H},\hat{N}] = 0 \xrightarrow{?} \hat{H}|n\rangle = E_n|n\rangle \tag{9}$$

Let us determine (hide all hat over operator)

$$[N,a] = a^\dagger aa - aa^\dagger a = (a^\dagger a - aa^\dagger)a = -a \tag{10}$$

$$\left[N,a^\dagger\right] = a^\dagger aa^\dagger - a^\dagger a^\dagger a = a^\dagger(aa^\dagger - a^\dagger a) = a^\dagger \tag{11}$$

Then determine

$$N(a|n\rangle) = (Na)|n\rangle = (aN - a)|n\rangle = (n-1)(a|n\rangle) \tag{12}$$

$$\to a|n\rangle = c_n|n-1\rangle = \sqrt{n}|n-1\rangle \tag{13}$$

$$\text{Since } \langle n|a^\dagger a|n\rangle = n\langle n|n\rangle = |c_n|^2\langle n-1|n-1\rangle \to c_n = \sqrt{n} \tag{14}$$

$$N(a^\dagger|n\rangle) = (Na^\dagger)|n\rangle = (a^\dagger + a^\dagger N)|n\rangle = (n+1)(a^\dagger|n\rangle) \tag{15}$$

$$\to a^\dagger|n\rangle = c_{n+1}|n+1\rangle = \sqrt{n+1}|n+1\rangle \tag{16}$$

$$\text{Since } \langle n|aa^\dagger|n\rangle = \langle n|(1+N)|n\rangle = (n+1)\langle n|n\rangle = |c_{n+1}|^2\langle n+1|n+1\rangle$$

$$\to c_{n+1} = \sqrt{n+1} \tag{17}$$

Note that a lower n steps by one and $a^\dagger$ increase n steps by one, so that n can be integer start from zero, i.e., $n = 0, 1, 2, 3, \ldots$. From (9), we get

$$E_n = \hbar\omega(n + 1/2),\ n = 0, 1, 2, \ldots \tag{18}$$

2.1.2 Fermi oscillator

Instead of (7), we rewrite the Hamiltonian in the form

$$H_F = \hbar\omega_F(N_F - \frac{1}{2}),\ N_F = c^\dagger c, \tag{19}$$

$$\{c, c^\dagger\} = 1, \{c, c\} = 0 = \{c^\dagger, c^\dagger\} \to c^2 = 0 = (c^\dagger)^2 \tag{20}$$

$$\overset{?}{\to} N_F|n_F\rangle = n_F|n_F\rangle \tag{21}$$

Let us determine

$$\{N_F, c\} = N_F c + cN_F = c^\dagger cc + cc^\dagger c = (c^\dagger c + cc^\dagger)c = c \tag{22}$$

$$\{N_F, c^\dagger\} = N_F c^\dagger + c^\dagger N_F = c^\dagger cc^\dagger + c^\dagger c^\dagger c = c^\dagger(c^\dagger c + cc^\dagger) = c^\dagger \tag{23}$$

Then determine

$$N_F(c|n_F\rangle) = (N_F c)|n_F\rangle = (c - cN_F)|n_F\rangle = (1 - n_F)(c|n_F\rangle) \tag{24}$$

$$N_F(c^\dagger|n_F\rangle) = (N_F c^\dagger)|n_F\rangle = (c^\dagger - c^\dagger N_F)|n_F\rangle = (1 - n_F)(c^\dagger|n_F\rangle) \tag{25}$$

We get similar action of $c, c^\dagger$ on $|n_F\rangle$, according to the action of N_F in (24, 25), let us assign

$$c^\dagger|0\rangle = |1\rangle,\ c^\dagger|1\rangle = 0 \to c|1\rangle = |0\rangle,\ c|0\rangle = 0 \tag{26}$$

So that $n_F = 0, 1$, restricted. From (19) we get

$$E_{n_F} = \begin{cases} +\frac{1}{2}\hbar\omega_F, & n_F = 1 \\ -\frac{1}{2}\hbar\omega_F, & n_F = 0 \end{cases} \tag{27}$$

Note that Fermi oscillator has no real classical analog system.

2.2 Second quantization

For a generic one particle Hamiltonian, together with its Schrodinger equation

$$H = \frac{p^2}{2m} + V(x) \to \left(-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)\psi(x) = E\psi(x) \tag{28}$$

$$E = \int d^3x\psi^*(x)\left(-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)\psi(x) \tag{29}$$

Second quantization is assigned, reinvent the hat for second quantized operators, in the form

$$E \to \hat{H},\ \psi(x) \to \hat{\psi}(x) = \sum_k \hat{a}_k\phi_k(x) \tag{30}$$

$$\int d^3x\phi_k^*(x)\phi_{k'}(x) = \delta_{kk'},\ \left(-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)\phi_k(x) = \epsilon_k\phi_k(x) \tag{31}$$

From (29), we get

$$\hat{H} = \sum_k \epsilon_k a_k^\dagger a_k \tag{32}$$

Note that a_k can be Bose or Fermi oscillator, it depends on a quantum particle we have described.

2.2.1 Tight-binding (TB) Hamiltonian

Schrodinger equation of an electron in periodic potential is

$$H = \frac{p^2}{2m} + V(r), \quad V(r+R) = V(r) \tag{33}$$

$$H\psi(r) = E\psi(r) \to E = \int d^3r\psi^*(r)H\psi(r) \tag{34}$$

where R is a lattice vector. Apply Bloch's theorem in the form

$$\psi(r) = \sum_j C_j e^{ik\cdot r}\phi_j(r),\ \phi_j(r+R) = \phi_j(r) \tag{35}$$

$$\begin{aligned}\to \psi(r+R) &= \sum_j C_j e^{ik\cdot(r+R)}\phi_j(r+R) \\ &= e^{ik\cdot R}\sum_j C_j e^{ik\cdot r}\phi_j(r) = e^{ik\cdot R}u(r)\end{aligned} \tag{36}$$

where $u(r+R) = u(r)$ is Bloch function, while $\phi_j(r)$ is localized Wannier function at the lattice site j. From (34) we will have

$$t_{ij} = -2\int d^3r \phi_i^*(r) H \psi_j(r),\ i,j = < i,j > \tag{37}$$

$$\to E = -\sum_{i,j} t_{ij}(C_j^* C_j + C_j^* C_i) = -t \sum_{<ij>} (C_i^* C_j + C^* j C_i) \tag{38}$$

Second quantization $C_i \to \hat{c}_i$, and $E \to \hat{H}$, then we have (after forget about the hat)

$$H = -t \sum_{<i,j>} (c_i^\dagger c_j + c_j^\dagger c_i),\ \text{with } j = i \pm 1 \tag{39}$$

This is the TB Hamiltonian. Let us rewrite

$$c_j = \frac{1}{\sqrt{N}} \sum_k e^{ikr_j} c_k \tag{40}$$

$$\begin{aligned} \sum_i c_i^\dagger c_{i\pm1} &= \frac{1}{N} \sum_i \sum_{k,k'} e^{-ik\cdot r_i + ik\cdot(r_i+R)} c_k^\dagger c_{k'} \\ &= \sum_{k,k'} c_k^\dagger c_{k'} e^{ik'\cdot R} \underbrace{\frac{1}{N}\sum_i e^{-i(k-k')\cdot r_i}}_{=\delta_{kk'}} = \sum_k e^{ik\cdot R} c_k^\dagger c_k \end{aligned} \tag{41}$$

From (39)

$$\begin{aligned} H = -t\sum_k \left(e^{ik\cdot R} c_k^\dagger c_k + h.c.\right) &= -t \sum_k \left(e^{ik\cdot R} + e^{-ik\cdot R}\right) c_k^\dagger c_k \\ &= \sum_k \epsilon_k c_k^\dagger c_k, \quad \epsilon_k = -2t\cos(k\cdot R) \end{aligned} \tag{42}$$

2.2.2 Magnetic systems

Magnetic system = localized spin lattice with Heisenberg interaction

$$H = -J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j \tag{43}$$

where $J > 0$ the system is ferro magnet, while $J < 0$ the system is anti-ferro magnet. (Other kinds magnetism are determined from loosely bound electron magnetic moments, see later on Stoner theorem.)

A single spin operator $\vec{S}^i$, $i = x, y, z$, can rewritten in second quantized form as

$$S^i = \frac{1}{2}\sum_{\alpha,\alpha'} c_\alpha^\dagger \sigma^i c_{\alpha'}, \tag{44}$$

where $\alpha = \{\uparrow, \downarrow\}$ is spin state, c_α is fermionic operator satisfy the algebra $\{c_\alpha, c_{\alpha'}^\dagger\} = \delta_{\alpha\alpha'}$, and σ^i is Pauli's matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},\ c_\alpha = \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$$

From (44) we have

$$S^x = \frac{1}{2}(c_\uparrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow) \tag{45}$$

$$S^y = \frac{1}{2}(c_\uparrow^\dagger c_\downarrow - c_\downarrow^\dagger c_\uparrow) \tag{46}$$

$$S^z = \frac{1}{2}(c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow) \tag{47}$$

The system of spins will be determined later.

2.3 Many-particle system

For a system N-particle with the Hamiltonian

$$H = \sum_{i=1}^{N} H_{0i} + \frac{1}{2}\sum_{i\neq j=1}^{N} V(r_i, r_j) \tag{48}$$

$$H_{0i} = \frac{p_i^2}{2m} + U(r_i) \tag{49}$$

when H_{0i} is one particle Hamiltonian, and $V(r_i, r_j)$ is two particle interaction potential. Its state function is written in generic form as

$$\psi_{\alpha_1\alpha_2...\alpha_N}(r_1, r_2, ..., r_N) = \mathcal{N}\sum_P \xi^P \varphi_{\alpha_1}(r_{P1})\varphi_{\alpha_2}(r_{P2})...\varphi_{\alpha_N}(r_{PN}) \tag{50}$$

$$\text{with} \int d^3r \varphi_\alpha(r)\varphi_\beta(r) = \delta_{\alpha\beta} \tag{51}$$

where $\mathcal{N}$ is the normalization factor, P is permutation, and ξ is statistical factor, $\xi = +1$ for bosonic system and $\xi = -1$ for fermionic system. For fermionic system $\psi_{\alpha_1...\alpha_N}(r_1,...,r_N)$ is written in term of Slater determinant. Schrodinger equation is

$$H\psi_{\alpha_1...\alpha_N}(r_1,...,r_N) = E_{\alpha_1...\alpha_N}\psi_{\alpha_1...\alpha_N}(r_1,...,r_N) \tag{52}$$

In one particle approximation, we have

$$E_{\alpha_1...\alpha_N} = \sum_{i=1}^{N}\epsilon_{\alpha_i} \tag{53}$$

One particle energy is

$$\begin{aligned}\epsilon = \sum_{\alpha}\epsilon_\alpha &= \sum_{\alpha}\int d^3r\varphi^*_\alpha(r)H_0\varphi_\alpha(r)\\ +\frac{1}{2}\sum_{\alpha,\beta}\int d^3r &\int d^3r'\varphi^*_\alpha(r)\varphi^*_\beta(r')V(r,r')\\ &\times\left\{\varphi_\beta(r')\varphi_\alpha(r)\pm\varphi_\beta(r)\varphi_\alpha(r')\right\}\end{aligned} \tag{54}$$

where+/$-$ signs mean bosonic/fermionic particle, and this is the *Fock (exchange) term*. The first part (direct) is called *Hartree term*.

Second quantization is apply by writing

$$\epsilon \to \hat{H},\ \ \varphi_\alpha(r) \to \hat{\varphi}_\alpha(r) = \sum_k \hat{a}_{k,\alpha}\phi_k(r),\ \ \int d^3r\phi^*_k(r)\phi_{k'}(r) = \delta_{kk'} \tag{55}$$

From (44), we will have

$$\int d^3r\varphi^*_\alpha(r)H_0\varphi_\alpha(r) = \sum_k \epsilon_k a^\dagger_{k,\alpha}a_{k,\alpha}, \tag{56}$$

$$\text{with}\ \ \epsilon_k\delta_{kk'} = \int d^3r\phi^*_k(r)H_0\phi_{k'}(r) \tag{57}$$

and with $\phi_k(r) = \frac{1}{\sqrt{V}}e^{ik\cdot r}$,

$$\begin{aligned}\int d^3r\int d^3r'\varphi^*_\alpha(r)\varphi^*_\beta(r')V(r-r')\varphi_\beta(r')\varphi_\alpha(r)&\\ = \frac{1}{V}\sum_{k,k',k'',k'''}\sum_q V(q)a^\dagger_{k'''}a^\dagger_{k''}a_{k'}a_k&\\ \times\frac{1}{V^2}\int d^3r\int d^3r' e^{-i(k'''-k-q)\cdot r}e^{-i(k''-k'+q)\cdot r'}&\\ = \frac{1}{V}\sum_{k,k',q}V(q)a^\dagger_{k+q}a^\dagger_{k'-q}a_{k'}a_k&\end{aligned} \tag{58}$$

The second quantized form of (54) is, forget the Hat,

$$H = \sum_{k,\alpha} \epsilon_{k,\alpha} a^{\dagger}_{k,\alpha} a_{k,\alpha} + \frac{1}{2V} \sum_{\alpha,\beta} \sum_{k,k',q} V(q) a^{\dagger}_{k+q} a^{\dagger}_{k'-q} \left(a_{k'} a_k \pm a_k a_{k'} \right) \tag{59}$$

Bosonic system

$$H_{boson} = \sum_{k,\alpha} \epsilon_{k,\alpha} b^{\dagger}_{k,\alpha} b_{k,\alpha} + \frac{1}{V} \sum_{\alpha,\beta} \sum_{k,k',q} V(q) b^{\dagger}_{k+q} b^{\dagger}_{k'-q} b_{k'} b_k \tag{60}$$

Fermionic system

$$H_{fermion} = \sum_{k,\alpha} \epsilon_{k,\alpha} c^{\dagger}_{k,\alpha} c_{k,\alpha} + \frac{1}{2V} \sum_{\alpha,\beta} \sum_{k,k',q} V(q) c^{\dagger}_{k+q} c^{\dagger}_{k'-q} (c_{k'} c_k - c_k c_{k'}) \tag{61}$$

2.3.1 Hubbard model

For system of strong interacting electrons, they are nearly localized from interaction. From (54) we can modified the second quantization in the form

$$\varphi_\alpha(r) = \sum_j c_{j,\alpha} \phi_j(r), \quad \int d^3 r \phi^*_j(r) \phi_{j'}(r) = \delta_{jj'} \tag{62}$$

Then we have

$$\begin{aligned} \int d^3 r \varphi_\alpha(r) H_0 \varphi_\alpha(r) &= \sum_{j,j'} c^{\dagger}_{j,\alpha} c_{j',\alpha} \underbrace{\int d^3 r \phi^*_j(r) H_0 \phi_{j'}(r)}_{=t_{ij},\ j,j'=<j,j'>} \\ &= \sum_j t_{ij} (c^{\dagger}_{j,\alpha} c_{j-1,\alpha} + h.c.) \rightarrow \text{"hopping"} \end{aligned} \tag{63}$$

$$\frac{1}{2V} \int d^3 r \int d^3 r' V(r,r') |\varphi_\alpha(r)^2 |\varphi_\beta(r')|^2 = U \sum_j n_{j,\alpha} n_{j,\beta} \tag{64}$$

It is the on site interaction term. So that (54) becomes

$$H = \sum_{j,\alpha} t_{ij} (c^{\dagger}_{j,\alpha} c_{j-1,\alpha} + h.c.) + U \sum_{j,\alpha,\beta} n_\alpha n_\beta \tag{65}$$

This is known as *Hubbard Hamiltonian*, according to J.C. Hubbard (1963).

2.4 Fock space

For a system of N-particle with n_i particles occupied in the i^{th} state and $n_i = 0, 1, 2, ...$ for boson and $n_1 = 0, 1$ for fermion. With the fact that $N = \sum_i n_i$, we can define number state of N-particle in the form

$$|N\rangle = |n_1\rangle \otimes |n_2\rangle \otimes ... = |n_1, n_2, ...\rangle \rightarrow \langle N|N'\rangle = \delta_{NN'} \tag{66}$$

We say that $|N\rangle$ span Fock space, the generalized Hilbert space as an infinite direct product of Hilbet space. This stat when acted by the annihilation/creation operators

$$a_i|n_1, n_2, ..., n_i, ...\rangle = (\pm)^{\sum_{j=1}^{i-1} n_j} \sqrt{n_i}|n_1, n_2, ..., n_i - 1, ...\rangle \tag{67}$$

$$a_i^\dagger|n_1, n_2, ..., n_i, ...\rangle = (\pm)^{\sum_{j=1}^{i-1} n_j} \sqrt{n_i + 1}|n_1, n_2, ..., n_i + 1, ...\rangle \tag{68}$$

According to the fact that

$$a_i|0\rangle = 0,\ a_i^\dagger|0\rangle = |1_i\rangle \rightarrow |1_i\rangle = \frac{a_i^\dagger}{1_i}|0\rangle \tag{69}$$

$$|2_i\rangle = \frac{(a_i^\dagger)^2}{2_i!}|0\rangle \tag{70}$$

$$|n_i\rangle = \frac{(a_i^\dagger)^n}{\sqrt{n_i!}}|0\rangle \tag{71}$$

$$|n_1, n_2, ..., n_i, ...\rangle = \frac{(a_1^\dagger)^n}{\sqrt{n_1!}}\frac{(a_2^\dagger)^n}{\sqrt{n_2!}}...\frac{(a_i^\dagger)^n}{\sqrt{n_i!}}...|0, 0, ..., 0, ...\rangle \tag{72}$$