Chapter 3: Hartree - Fock Approximation.

- P. Phillips book
- G. Giuliani & G. Vignale book.

Hartree-Fock theory was developed in the 1930-1940 time for solving few body problems, such as He-atom that we have studied in QM-II course. Its a variational method to solve for the ground state of a many body system by expressing the trial wave function in the basis of single-particle "product state." The single particle states are the variational parameters. Clearly, this assumption of single particle product state (which is exact for an non-interacting system) is flaw. But it seems to work quite well for weakly interacting system. This H-F. method is used in the density functional theory (DFT) calculation, and it turns out to be quite accurate to describe the band structure picture of weakly correlated electron systems.

The Hamiltonian we have is

$$H = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 - Ze^2 \underbrace{\sum_{i,I}\frac{1}{|\vec{r}_i - \vec{R}_I|}}_{v_{ie}(r_i)} + \frac{e^2}{2}\underbrace{\sum_{i\neq j}\frac{1}{|\vec{r}_i - \vec{r}_j|}}_{v_{ee}(\vec{r}_i - \vec{r}_j)} \quad -(1)$$

(denote)

We will first look at it in the 1st quantized formalism for fermions. Here we have a slater determinant as the trial wave function in terms of single particle wavefunction $u_\alpha(\vec{r}_i)$. We wrote it in the previous chapter. Then the total energy of the Hamiltonian is easily obtained to be

$$E_G = \langle G|H|G\rangle = -\frac{\hbar^2}{2m}\sum_\alpha \int |\nabla u_\alpha|^2 d^3r + \int d^3r\, v_{ie}(\vec{r})\,|u_\alpha|^2$$

$$+ \frac{1}{2}\sum_{\alpha\neq\beta}\int d^3r\, d^3r'\, |u_\alpha(\vec{r})|^2\, v_{ee}(\vec{r}-\vec{r}')\,|u_\beta(r)|^2$$

"direct term"/ Hartree term

$$- \frac{1}{2}\sum_{\alpha\neq\beta}\int d^3\vec{r}\, d^3\vec{r}'\, u^*_\alpha(\vec{r})\, u^*_\beta(\vec{r}')\, v(\vec{r}-\vec{r}')\, u_\alpha(\vec{r}')\, u_\beta(\vec{r})$$

"Exchange term"/ Fock term. --②.

<u>H.W.</u> Solve for eq ② from eq ① for two particles's wavefunction

$$|G\rangle \equiv \Psi(r_1, r_2) = \frac{1}{\sqrt{2}}\Big[\underbrace{u_\alpha(r_1)\, u_\beta(r_2)}_{\text{Term 1}} - \underbrace{u_\alpha(r_2)\, u_\beta(r_1)}_{\text{Term 2.}}\Big]$$

The first two terms are the single particle terms and are easily obtained by virtue of the orthogonalization property of the u_α states. The third term, called the direct term, arises from the expectation value of the $\langle \text{Term 1}|V_{ee}|\text{Term 1}\rangle = \langle \text{Term 2}|V_{ee}|\text{Term 2}\rangle$, which depends on the probability densities $|u_\alpha|^2$, $|u_\beta|^2$ of the wavefunction. It does not depend on the phase of the wavefunctions, so, its like a classical term. The last term, called the exchange term, arises from the $\langle \text{Term 1}|V_{ee}|\text{Term 2}\rangle = \langle \text{Term 2}|V_{ee}|\text{Term 1}\rangle^*$. This actually arises due to the superposition principle of the wavefunction and for the exchange statistics of quantum particles. The term also depends on the phase & amplitude of each wave functions. Therefore, its a proper quantum term.

The idea is to treat the single particle states $u_\alpha(\vec{r})$ as variational parameters. By varying $u_\alpha(\vec{r})$ we may obtain a minimum E_G. However, the new $u_\alpha(\vec{r})$ are no longer the eigenstate of the first two non-interacting terms. It may be an eigenstate of some other fictitious single particle Hamiltonian, which we don't care. But the physical interpretation is that in a many body system, due to interaction the single electron's state is modified with different effective mass, possibly different screened charge, etc. But its single particle identity remains valid, and the states are possibly adiabatically connected to the original single particle state - although this is not a criterion in the Hartree-Fock approximation.

In the direct/Hartree term, the particles in states α & β before the two-body interaction remains in their same α, β- states after the interaction and we sum over all possible states α & β at all possible positions $\vec{r}, \vec{r}'$. This term depends on density $|u_\alpha|^2$, not on phase.

The exchange/Fock term comes with a negative sign - which comes from the antisymmetry wave function. In this case, the two particles exchange their states during the two-body interaction. This is an important term because of which quantum magnet exists which one can see by including the spin index in the α- index. The exchange term has no classical probabilistic interpretation as in the direct term and is purely arising from the quantum statistic of the particle. It also has a negative sign for fermions. This term is usually very very small, compared to the direct term. Because, suppose, two particles are far far away from each other, then the overlap of the two wavefunctions u_α & u_β at $\vec{r}_1 >> \vec{r}_2$ is very very small. This is the reason, classically when the two particles are well separated, this term is zero. When the two state wavefunctions are close enough to overlap, the exchange term gives finite contribution. This term starts to dominate when the wavefunctions starts to overlapp, ie, when there is a finite probability that two particles are present at the same position. This term also depends on the full wavefunction, $u_\alpha(\vec{r})$, while the direct term depends on its amplitude only.

The variation process is $\frac{\delta E_n[\phi_\alpha]}{\delta u_\alpha} = 0, \ \forall \alpha$.

In the variational process, as we vary u_α, we have to ensure that the states $u_\alpha(\vec{r})$ remain mutually orthonormalized as this was our fundamental assumption to begin with. The constraint is

$$\int d^3r \, u^*_\alpha(r) \, u_\beta(r) = \delta_{\alpha\beta}. \quad ---(3)$$

This constraint is added to the functional minimizations of E_n in eq(2) by a Lagrangian multiplier ε. One may think of adding $\varepsilon_{\alpha\beta}$ - multiplier for the whole matrix in eq(3). But it turns out one does not need such a N×N matrix, u_α are automatically orthonormal, and its only the normalization constraint for each state that one needs to impose. So, a diagonal ε_α is required here. Once we put ε_α multipliers to impose eq(3) constraint to eq ② and do the variational derivative w.r.to ϕ_α, we obtain linearized eigenvalue equations of an effective Hamiltonian - called the Hartree-Fock Hamiltonian with ε_α being the corresponding eigenvalues:

$$H_{HF}|u_\alpha\rangle = \varepsilon_\alpha |u_\alpha\rangle \quad --(4).$$

where ε_α is called the Hartree-Fock energy, or quasiparticle (single-particle) energy.

$$\text{where} \quad H_{HF}(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2 + v_{ie}(\vec{r}) + V_H(\vec{r}) + V_{ex}(\vec{r}) \quad -(5a)$$

$$\text{with} \quad V_H(r) = \int d^3\vec{r}\,' \sum_\beta |u_\beta|^2(\vec{r}\,')\, v_{ee}(\vec{r}-\vec{r}\,') = \text{Hartree energy} \quad -(5b)$$

$$V_{ex}(\vec{r}-\vec{r}\,') = V_F(r-\vec{r}\,') = \sum_\beta u^*_\beta(\vec{r}\,')\, u_\beta(\vec{r})\, v_{ee}(\vec{r}-\vec{r}\,'). \quad --(5c)$$

$$= \text{Exchange / Fock energy}$$

Note that this is a non-local potential, which depends on ϕ_α.

H.W. Derive eq ④ & ⑤ from eq ② & ③.

So Hartree-potential is some effective potential seen by the α-quasiparticle due to other quasiparticles interacting with α. quasiparticle locally. One picks a different position $\vec{r}\,'$, and put a classical probability of having another particle $|u_\beta|^2$ at that position which interacts with α particle by $v(\vec{r}-\vec{r}\,') \sim e^2/|\vec{r}-\vec{r}\,'|$, and then integrate over $\vec{r}\,'$ and sum over all states $\beta \neq \alpha$. It's a classical probability because the phase of the wavefunction u_β does not contribute to the Hartree energy. But the identical particle concept of quantum mechanics gives you the exchange term - which depends on the phase difference between the state u_β at two different positions $\vec{r}, \vec{r}\,'$, and depends on the quantum statistics and interference.

We actually <u>don't</u> quite have a linear eigenvalue eq (time-independent Schrödinger equation), rather a slightly modified one as

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ie} + V_H(r)\right] u_\alpha(\vec r) + \int d^3\vec r\,' \underbrace{V_F(\vec r - \vec r\,')\, u_\alpha(\vec r\,')}_{u_\alpha \text{ depends on } \vec r\,',\text{ not } \vec r.}$$

$$= \varepsilon_\alpha u_\alpha(\vec r). \qquad \longrightarrow (6).$$

This is like a non-linear Schrödinger equation. So, one cannot solve it as a eigenvalue equation, but one needs to solve it self-consistently. One first gauss the solution $u_\alpha(\vec r)$ and then evaluate the potentials V_H, V_{ex}, and then solve for new $u_\alpha(\vec r)$, until the gauss and evaluated ϕ_α match with each other with accepted accuracy. ε_α are the single particle excitation energy - this is the amount of energy required to be added or subtracted from the total energy if we add or remove a particle.

⊛ This was the crucial part of the Hartree-Fock theory that an interacting Hamiltonian turns into a single-particle Hamiltonian - as if the quasiparticles are moving in an effective potential due to other quasiparticles. The crux of approximation, of course, lies in the wave function. Generally, a product of single-particle state forms a proper basis state and one can expand a many body state in this basis as

$$\Psi(r_1 \cdots r_N) = \sum_{\alpha_1 \cdots \alpha_N} C_{\alpha_1 \cdots \alpha_N}^{(r_1 \cdots r_N)}\, u_{\alpha_1}(r_1) \cdots u_{\alpha_N}(r_N)$$

where $C_{\alpha_1 \cdots \alpha_N}$ are complex coefficients for each permutation. This is a general state. But the approximation lies in setting $C_{\alpha_1 \cdots \alpha_N} = \pm 1$ for all basis states. There are other complicated states, such as matrix product state, tensor product states that can be built from this general state which can include entanglement, fractionalization, topological properties, that one may learn in other courses. The assumption here that many body ground state is a linear superposition of all possible permutations of single particle product state with equal probability, i.e, $|c_{\alpha_1 \cdots \alpha_N}|^2=1$ in the H.F. approximation. The advantage of a product state is that it helps split the Hamiltonian into a direct sum of Hamiltonians whose eigenvalues are the components of the product states. This approximation works fairly well at the weak coupling limits and in many magnets, but believe to fail near a phase transition, or in the case of Mott insulator etc.

Hartree-Fock Theory in Second Quantization
- A Mean Field Theory.

We will now derive the Hartree-Fock theory in second quantized formalism, and learn that the decomposition of the two-body interaction term into the single-body effective Hamiltonian is similar to the socalled mean-field theory or the Wick's theory. The theory is general to any interacting Hamiltonian and for bosons & fermions. We will start with the same many-body Hamiltonian as before and at the end we will redo the formalism for a general case.

We split the Hamiltonian (eq1) into a single-particle (one body) and interaction (two-body) term as

$$H = H_1 + H_2, \text{ where } H_1 = T + V_{ie}, \; H_2 = V_{ee}. \quad \text{--} ⑦$$

This can be expressed in second quantization as

$$\mathcal{H}_1 = \sum_{\alpha\beta} \underbrace{\langle\alpha| H_1 |\beta\rangle}_{h_{\alpha\beta}} c^{+}_{\alpha} c_{\beta} \quad \text{---} (8a)$$

$$\mathcal{H}_2 = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} \, c^{+}_{\alpha} c^{+}_{\beta} c_{\delta} c_{\gamma} \quad \text{---} (8b)$$

$$\text{where } h_{\alpha\beta} = \langle\alpha| \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{ie}(\bar{r}) \right] |\beta\rangle,$$

$$= \int d^3r \, u^{*}_{\alpha}(r) \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{ie}(r) \right] u_{\beta}(r); \quad \text{--} (8c)$$

and $v_{\alpha\beta\gamma\delta} = \langle \alpha\beta \,|\, v_{ee}(\vec{r}-\vec{r}') \,|\, \gamma\delta \rangle$

$$= \int d^3r\, d^3r'\; u^*_{\alpha}(r)\, u^*_{\beta}(r')\; v_{ee}(\vec{r}-\vec{r}')\, u_{\gamma}(\vec{r}')\, u_{\delta}(\vec{r}) . \quad \text{---} \quad (8d)$$

- The one body term can be interpreted as a particle in tunneling from the state β to α at an energy cost $(H_1)_{\alpha\beta}$. This term, in general, is not diagonal, depends on the basis one choses. For example, if α, β are the Wannier basis, then one can have an electron hopping from β-site to α-site. Then by doing the Fourier transformation to the momentum space one obtains a diagonal one-body term as

$$\mathcal{H}_1 = \frac{1}{V} \sum_{\substack{\alpha,\beta \\ k,k'}} \langle k | H_1 | k' \rangle\, e^{i(\vec{k}'\cdot\vec{r}_\beta - \vec{k}\cdot\vec{r}_\alpha)}\, c^\dagger_k c_{k'} \quad \text{--} \quad (9a)$$

Now, $\vec{r}_\beta - \vec{r}_\alpha = \delta$ = distances between nearest neighbors. We take only first nearest neighbor for simplicity

$$= \frac{1}{V} \sum_{\substack{\alpha,\beta \\ k,k'}} \langle k | H_1 | k' \rangle\, e^{i(\vec{k}'-\vec{k})\cdot\vec{r}_\alpha} \cdot e^{i\vec{k}'\cdot\delta}\, c^\dagger_k c_{k'}$$

The α-summation $= \frac{1}{V}\sum_{\alpha} e^{i(\vec{k}'-\vec{k})\cdot\vec{r}_\alpha} = \delta_{k,k'}$. Then defining $\varepsilon_k = \langle k | H_1 | k \rangle\, e^{i\vec{k}\cdot\delta}$ as the quasi-particle energy with the k-wavevector. Then the Hamiltonian is diagonal in the k-space

$$\langle G | H_1 | G \rangle = \sum_k \varepsilon_k\, \underbrace{c^\dagger_k c_k}_{n_k} . \quad \text{---} \quad (9b)$$

If on the other hand, α, β corresponds to orbital/spin/sublattice indices, then $H_{\alpha\beta}$-term has off-diagonal elements. One needs to diagonalize it and obtain quasiparticle energy. For α, β being combination of wannier site index and orbital indices, the Fourier transformation to momentum space will diagonalize the site index, and one then diagonalize the orbital part.

- The interaction term is normal ordered as $c^\dagger c^\dagger c c$ as convention. The ordering between γ, δ in H_2 and that in 'C' are reversed, which otherwise amounts to a negative sign. This gives a scattering term with two quasiparticles going from γ, δ-states to α, β-states. Assuming $\alpha, \beta, \gamma, \delta$ indices to be wannier sites, we do Fourier transform to the momentum space:

$$\mathcal{H}_2 = \frac{1}{V^2} \sum_{\substack{\alpha\beta\gamma\delta, \\ k_1 k_2 k_3 k_4}} \underbrace{\langle k_1 k_2 | H_2 | k_3 k_4 \rangle}_{V_{k_1, k_2, k_3, k_4}} e^{i(\vec{k}_1 \cdot \vec{r}_\gamma + \vec{k}_2 \cdot \vec{r}_\delta - \vec{k}_3 \cdot \vec{r}_\alpha - \vec{k}_4 \cdot \vec{r}_\beta)} c^\dagger_{k_3} c^\dagger_{k_4} c_{k_2} c_{k_1} \quad \text{--(9c)}$$

Now, assuming that translational symmetry remains valid in this scattering process, the total momentum remains conserved, i.e.,

$$\vec{k}_1 + \vec{k}_2 = \vec{k}_3 + \vec{k}_4 = -\vec{q} \quad (\text{defined})$$

This momentum conservation condition removes one of the momentum variables, and we have

$$\mathcal{H}_2 = \sum_{k, k', q} V_{k, k', q} \, c^\dagger_k c^\dagger_{k'} c_{k'-q} c_{k+q} \quad \text{---(9d)}$$

With orbital/spin indices, its the same game as we discussed for the one-body term.

$$H_2 = \sum_{k, k', q} V^{\alpha\beta\gamma\delta, \sigma\sigma'\sigma''}_{k k' q} c^\dagger_{k\alpha\sigma} c^\dagger_{k'\beta\sigma''} c_{k-q\delta\sigma'''} c_{k+q\gamma\sigma'}$$

⊛ Now we will evaluate the matrix-element of the 2nd quantized Hamiltonian with respect to the H. F. wavefunction in the 2nd quantization for fermions.

$$|G\rangle = \prod_{\substack{\nu \\ \varepsilon_\nu < \mu}} c_\nu^\dagger |0\rangle \quad \text{---} (10)$$, where $\mu =$ chemical pot.

This state is the same as the slater-determinant state, where $c_\alpha^\dagger|0\rangle$ corresponds to α-state being occupied if its quasiparticle energy lies below the Fermi level. The anti-symmetry part is captured by the anti-commutation between c_α's..

$$\Rightarrow \langle G|H_1|G\rangle = \langle 0|\prod_\nu c_\nu \Big| \sum_{\alpha\beta} h_{\alpha\beta}\, c_\alpha^\dagger c_\beta \Big| \prod_\eta c_\eta^\dagger |0\rangle$$

- $$c_\beta \, \underbrace{| \text{---} \, c_\beta^\dagger \cdots |0\rangle}_{|\cdots\, n_\beta \,\cdots\rangle} = \sqrt{n_\beta}\; \zeta^{\sum_{i=1}^{\beta-1} n_i} \,|\cdots\, n_\beta - 1 \cdots\rangle$$

- $c_\alpha^\dagger |\cdots\, n_\beta - 1 \cdots\rangle = ?$ Note that in the bra state we have all the states filled. Therefore, after the action of $c_\alpha^\dagger$, the ket state has to be same as the bra state. This means, the only term that contribute here is when $\alpha = \beta$. So, we have
$$c_\alpha^\dagger |\cdots\, n_{\beta-1} \cdots\rangle = \sqrt{n_\beta}\; \zeta^{\sum_{i=1}^{\beta-1} n_i} \,|\cdots\, n_\beta \cdots\rangle$$

- Hence, in this basis the non-interacting term is diagonal. We get.
$$\langle G|H_1|G\rangle = \sum_\alpha h_{\alpha\alpha} \underbrace{n_\alpha}_{n_\alpha = 1 \text{ for } \varepsilon_\alpha < \mu} = \mathrm{Tr}\, \hat{h}. \quad \text{---} (11)$$

Note that we have not yet defined what is ε_α, we will define it below.

where $h_{\alpha\alpha} = \int d^3r \; u_\alpha^*(r)\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ion}^{(r)}\right] u_\alpha(r)$

$$= \int d^3r \left[\frac{\hbar^2}{2m}|\vec{\nabla} u_\alpha|^2 + V_{ion}(r)\,|u_\alpha|^2\right]$$

as in the 1st quantized form.

$$\Rightarrow \langle G|H_2|G\rangle = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|v_{ee}|\gamma\delta\rangle \times$$

$$\langle 0|\cdots c_\alpha \cdots c_\beta \,|\, c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \,|\, \cdots c_\gamma^\dagger \cdots c_\delta^\dagger \cdots |0\rangle$$

- $c_\delta c_\gamma |\cdots c_\gamma^\dagger \cdots c_\delta^\dagger \cdots |0\rangle = \sqrt{n_\delta}\sqrt{n_\gamma}\; \mathcal{J}^{\sum_{i=\gamma}^{\delta} n_i} |\cdots n_\gamma - 1 \cdots n_\delta - 1 \cdots\rangle$ for $\delta > \gamma$
- $c_\alpha^\dagger c_\beta^\dagger |\cdots n_\gamma - 1 \cdots n_\delta - 1 \cdots\rangle = ?$

For the same reason, as before, we have two options here: $\alpha = \delta, \beta = \gamma$ or $\alpha = \gamma, \beta = \delta$. The 2nd term has a negative sign due to the fact that we need to bring $c_\alpha^\dagger$ state before $c_\beta^\dagger$ as $c_\alpha^\dagger c_\beta^\dagger \to - c_\beta^\dagger c_\alpha^\dagger$ for $c_\alpha^\dagger$ state to act on γ-state first. So we get

$$= (\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta})\sqrt{n_\delta}\sqrt{n_\gamma}\; \mathcal{J}^{\sum_{i=\gamma}^{\delta} n_i} |\cdots n_\gamma \cdots n_\delta \cdots\rangle$$

Therefore we get

$$\langle G|H_2|G\rangle = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} (v_{ee})_{\alpha\beta\gamma\delta}\left(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\gamma}\right) n_\gamma n_\beta$$

$$= \sum_{\alpha\neq\beta}\left[(v_{ee})_{\alpha\beta\alpha\beta} - (v_{ee})_{\alpha\beta\beta\gamma}\right] n_\alpha n_\beta \qquad \cdots (12)$$

where

$$(v_e)_{\alpha\beta\alpha\beta} = \int d^3r\, d^3r'\, u^*_\alpha(r)\, u^*_\beta(r')\, v_{ee}(\vec{r}-\vec{r}')\, u_\alpha(r)\, u_\beta(r')$$

$$= \int d^3r\, d^3r'\, v_{ee}(\vec{r}-\vec{r}')\, |u_\alpha(r)|^2\, |u_\beta(r')|^2 .$$

$=$ Direct / Hartree term. $\equiv V_{\alpha\beta}$ --- (13a)

$$(v_e)_{\alpha\beta\beta\alpha} = \int d^3r\, d^3r'\, u^*_\alpha(r)\, u^*_\beta(r')\, v_{ee}(\vec{r}-\vec{r}')\, u_\beta(r)\, u_\alpha(r')$$

$=$ Exchange / Fock term $= J_{\alpha\beta} = J_{\beta\alpha}$

(The exchange term is often denoted by J). --(13b)

These results are same as what we obtained via first quantization.

- Therefore, the H.F. approximation allows us to decouple the interaction term into a single particle (not the same atomic electrons that started with, but quasiparticle with dressed energy ε_α) Hamiltonian, in which the dressed quasiparticles interact with average potential caused by other quasiparticles (direct term) and also a quantum mechanical (exchange) term in which the identical quasiparticle exchanges its state during the interaction. Another way to say, in the H.F. theory one only keeps the density-density interaction term and ignore all other interaction/scattering processes.
- This results in an effective non-interacting Hamiltonian which can be expressed as

$$\mathcal{H} = \sum_\alpha \varepsilon_\alpha \tilde{a}^\dagger_\alpha \tilde{a}_\alpha ,$$ where ε_α is the quasiparticle excitation energy, and $\tilde{a}_\alpha$ are the quasiparticle destruction operator, which acts on the Fermi-sea $|G\rangle$. ε_α energy is required to be added (subtracted to the total energy to add or remove a quasiparticle. This was first proposed by Koopman, and this way of thinking about the quasiparticle excitation is called the Koopman theorem.

H.W. ① Recalculate eqs (11), ⑫ by considering the spin explicitly as $\alpha \equiv \alpha, \sigma$, where $\sigma = \uparrow, \downarrow$. Show that the non-interacting term and the direct term are spin degenerate terms, while the exchange term involves a spin flip as $H_{ex} \sim \sum_{\substack{\alpha\beta \\ \sigma, \sigma'}} J_{\alpha\beta} \, n_{\alpha\sigma} \, n_{\beta\sigma'}$.

(2) Repeat the same exercise for $\alpha = i, \alpha, \sigma$, where $i =$ unit cell index, $\alpha =$ orbital / sublattice index, and $\sigma = \uparrow, \downarrow$ index.

(3) Now Fourier transform the exercise (2) to the momentum space.

⊛ Correspondence between the H. F. theory and the Wick's theorem – They are all mean-field theories.

The key lesson of the H.F. theory is that one can split an interacting Hamiltonian into a product of two quasiparticle densities if one starts with a many body state in terms of single particle state. Writting inversly, if one starts with single particle states and compute the expectation value of an interaction term, the interaction term breaks into a product of single-particle term. A single-particle term means – in second quantization – a term made of 'a^+a' or quadratic in terms of creation/annihilation operators (In field theory, a quadractic term is also called a Gaussian term). Then an interaction term a^+b^+cd breaks into expectation values of all possible quadratic terms as

$$\langle a^+b^+cd\rangle = \langle a^+d\rangle\langle b^+c\rangle - \langle a^+c\rangle\langle b^+d\rangle.$$

where the expectation value is taken in a single-particle (quadratic) ground state. The first term is the direct term and the second term is the exchange term, which a negative sign which arises due to odd-number of fermionic exchanges. This was shown by Wick and called the Wick's theorem.

This theory is greatly useful in the perturbation theory, where we consider the non-interacting (quadratic) Hamiltonian as the non-perturbative part, and compute the interaction part as perturbation. Then in all perturbation terms the interaction term arises with even number of a^+a. The expectation value of these terms in terms of non-interacting unperturbed state always breaks down into products of qudractic terms. This way we can solve the perturbation series.

This H.F. or Wick theory is also used in the so-called Mean-field theory. In the mean field theory, we assume in the ground state the mean value of the quadratic terms (such as densities) exist and then we consider slight variations around the mean values to obtain the low-energy excitations. Mathematically, we write them as $a^\dagger a \simeq \langle a^\dagger a\rangle + \tilde{a}^\dagger \tilde{a}$, where $\tilde{a}$ is the annihilation of a quasiparticle on the mean-field ground state. (Sometimes we insert : : to emphasize that $\tilde{a}^\dagger, \tilde{a}$ operators are defined with respect to the ground state, i.e, they are the excitations whose vacuum state is the ground-state).

$\langle a^\dagger b^\dagger b a\rangle = \langle a^\dagger a\rangle \langle b^\dagger b\rangle$, and $\langle a^\dagger b\rangle = \langle b^\dagger a\rangle = 0$ in the ground state.

$$\& \quad a^\dagger b^\dagger b a \approx \text{like } (\underbrace{\langle a^\dagger a\rangle + \tilde{a}^\dagger\tilde{a}}_{\langle\phi\rangle - \delta\phi})(\underbrace{\langle b^\dagger b\rangle + \tilde{b}^\dagger\tilde{b}}_{\langle\psi\rangle - \delta\psi})$$

excitations above mean field ground state

$$\approx \underbrace{\underbrace{\langle a^\dagger a\rangle\langle b^\dagger b\rangle}_{\langle\phi\rangle\langle\psi\rangle}}_{\text{Ground state energy.}} + \underbrace{\underbrace{\langle a^\dagger a\rangle\, \tilde{b}^\dagger\tilde{b}}_{\langle\phi\rangle\,\delta\psi} + \underbrace{\langle b^\dagger b\rangle\, \tilde{a}^\dagger\tilde{a}}_{\langle\psi\rangle\,\delta\phi}}_{\text{Single-particle/quadratic excitations above the ground state.}} + \underbrace{\tilde{a}^\dagger\tilde{a}\,\tilde{b}^\dagger\tilde{b}}_{+(\delta\phi)(\delta\psi)\text{ ignore it as its small.}}$$

$$\approx \langle a^\dagger a\rangle\, \tilde{b}^\dagger\tilde{b} + \langle b^\dagger b\rangle\, \tilde{a}^\dagger\tilde{a} + \langle a^\dagger a\rangle\langle b^\dagger b\rangle \quad \text{— (14).}$$

We can re-express $\tilde{a}, \tilde{b}$ operators in terms of a, b as $\tilde{a}^\dagger\tilde{a} = a^\dagger a - \langle a^\dagger a\rangle$ & $\tilde{b}^\dagger\tilde{b} = b^\dagger b - \langle b^\dagger b\rangle$. Substituting them in eq (14) we get

$$a^\dagger b^\dagger b a \approx -\langle a^\dagger a\rangle\langle b^\dagger b\rangle + \langle a^\dagger a\rangle b^\dagger b - \langle b^\dagger b\rangle\langle a^\dagger a\rangle - \langle b^\dagger b\rangle a^\dagger a$$
$$+ \langle a^\dagger a\rangle\langle b^\dagger b\rangle$$
$$= \langle a^\dagger a\rangle b^\dagger b + \langle b^\dagger b\rangle a^\dagger a - \langle a^\dagger a\rangle\langle b^\dagger b\rangle . \quad -(15)$$

This is the equation we will be using throughout this course. The interpretation of eq (15) is very similar to the Hartree-Fock equation that although the left hand side is an interaction term, we approximate it as each particle see all other particles providing a mean-field density to it. In the above case, we have set another mean field term $\langle a^\dagger b\rangle$ only for simplicity, otherwise this term should also be included and one will obtain two mean-field potential as

$$a^\dagger b^\dagger b a \approx \langle a^\dagger a\rangle b^\dagger b + \langle b^\dagger b\rangle a^\dagger a + \langle a^\dagger b\rangle b^\dagger a + \langle b^\dagger a\rangle a^\dagger b$$
$$- \langle a^\dagger a\rangle\langle b^\dagger b\rangle - \langle a^\dagger b\rangle\langle b^\dagger a\rangle .$$

The expectation value of each mean-fields $\langle a^\dagger a\rangle$, $\langle b^\dagger b\rangle$ $\langle a^\dagger b\rangle$, $\langle b^\dagger a\rangle$ are calculated self-consistently. We have done a similar self-consistent mean field theory in Advanced Statistical Physics course for the Ising model. We will employ the mean-field theory in Chapter 6 & 7 for the Hubbard model and for superconductivity.