Chapter 2: Second Quantization

We will continue to solve the electronic and nucleous parts of the Hamiltonian for the electron-electron interaction and phonon, but we will use a simpler notations to express the Hamiltonians. The second quantization method does not introduce any approximation or method to the many body condensed matter problem we study here. It is infact more general and used in other theories. It simply changes the language and perspective of the problem and, in most cases, make it easier to study and understand the quantum theory.

Our ultimate goal is to solve for many-body states. In the absence of any exact solution, we often resort to the variational or mean field theory. In both cases, we essentially solve for an effective single-particle wavefunction moving under the mean-values of potential provided by all other particles. Then we construct a many body wavefunction as a product state of these single quasiparticles. We, however, have to incorporate the quantum symmetry, called the permutation symmetry of particles in this state. Simply speaking, the wavefunction has to be symmetric (anti-symmetric) for bosons/ fermions.

We will first review the first quantization procedure, in which we consider each particle and solve for their eigenstate. In the second quantization procedure, we change our perspective. We solve for states and then ask how many particles occupy that state. For the case of identical particle, the 2nd procedure simplify the problem.

First Quantization :

Before we introduce the second quantization procedure, let us first review what is the first quantization. This is something we studied in quantum mechanics course, where we have a Hamiltonian written in terms of the coordinates of the particles. Then we quantize the theory by solving the Schrödinger equation with boundary condition, orthonormalization condition. This gives us the quantum numbers and energy eigenstates of the Hamiltonian at hand. So, we have a Hilbert space of the energy eigenstates which depends on the Hamiltonian.

In 1st quantization, we have fixed number of particle, say N. We look into each particle's coordinate $\bar{r}_i$, and momentum $\bar{p}_i$, and write a wavefunction in each particle's position (or momentum space). To be general, we will index the basis states by α, which can be energy basis ($\equiv n$), momentum ($\equiv k$), angular momentum ($\equiv l$), and/or sublattice/spin etc. Let $u_\alpha(r_i) = \langle r_i|\alpha\rangle$ are such states for the i^{th} particle. $u_\alpha(r_i)$ can be the eigenstate of the single particle Hamiltonian $h(r_i)$: $h(r_i)\, u_\alpha(r_i) = e_\alpha\, u_\alpha(r_i)$, or momentum eigenstate $p_i\, u_k(r_i) = \hbar k\, u_k(r_i)$, and so on. $u_\alpha(r_i)$ are orthonormalized

$$\int d^3r_i \; u_\alpha^*(r_i)\, u_\beta(r_i) = \delta_{\alpha\beta} .$$

They form a complete set $\sum_\alpha |\alpha\rangle\langle\alpha| = \mathbb{I} = \sum_\alpha \int d^3r_i \langle r_i|\alpha\rangle\langle\alpha|r_i\rangle$
$= \sum_\alpha \int d^3r_i \; u_\alpha^*(r_i)\, u_\alpha(r_i)$.

Therefore, the general solution for the single particle state at $\bar{r}_i$ is

$$u(r_i, t) = \sum_\alpha a_\alpha(t)\, u_\alpha(\bar{r}_i),$$ where

$a_\alpha(t) = a_\alpha(0)\, e^{-i e_\alpha t/\hbar}$, if $u_\alpha(r_i)$ are the eigenstates of $h(r_i)$.

⊛ Many-body state for N-particles:

Assuming an independent (non-interacting) particles picture, the full Hamiltonian can be split into a direct sum of single particle one

$$H(r_1, \cdots, r_N) = \bigoplus_{i=1}^{N} h(r_i) = \sum_{i=1}^{N} h(r_i). \quad \text{--(1)}$$

where $h(r_i) = -\frac{\hbar^2}{2m}\nabla_i^2 + V_{Ie}(r_i)$.

The solution of this Hamiltonian is a simple product state

$$\Psi(r_1; \cdots; r_N) = u_{\alpha_1}(r_1)\, u_{\alpha_2}(r_2) \cdots u_{\alpha_N}(r_N). \quad \text{--(2).}$$

Since $u_{\alpha_i}(r_i)$ are orthonormal, complete basis states, so Ψ is also orthonormal and form a Hilbert space.

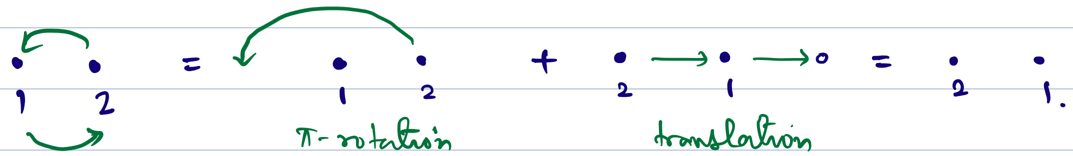
Identical Particles and Statistics

As a quantum many-body state eq (2) is not enough as it does not satisfy an important exchange symmetry of quantum identical particles. Because of the exchange symmetry, any two particles are indistinguishable or identical. In other words, identical particles result from the exchange symmetry, which says, the system is invariant under the exchange of two particles. For a system of many particles, an operator that exchanges two particles, swapping their position/state, leaves the physics invariant. This symmetry is represented by a unitary transformation acting on the many-body wavefunction. We denote it by

$$P\,\Psi(1,2) = e^{i\theta}\,\Psi(2,1), \quad \text{—(3).}$$

where we have added a phase 'θ' for future use.

It turns out that the exchange between two identical particles is same as wraping one particle by π and the translate it



- In 2D, both particles lie on the same x-y plane. So, rotation of particle 2 with respect to 1 makes it not a simply connected path. Because, as we rotate 2 around 1, this path cannot be contracted to vanish to a point. Because, the particle 1 is always there inside the contour. Therefore, an exchange in 2D makes the complex wave-function a multivalued function, living on a multiple Reimann sheet and has branch cut. Therefore, the wavefunction can differ by a phase $e^{i\theta}$ upon 2π rotation, and one needs to rotate it n-times such that $\theta = 2n\pi$, or exchange it $2n$-times to have the wavefunction return to itself. Here the exchange of the particles follow a permutation group. This is called Abelian (commuting) anyons.
If the wavefunction has N-fold degeneracy (and/or a N-component spinor), the exchange can rotate the wavefunction in the manifold as $\psi_a = [\gamma]_{ab}\psi_b$. Then if γ-matrices do not commute, then the corresponding particles are called non-Abelian anyons. They follow Braid group.

3D: In 3D, the exchange also follow the permutation group, but has two elements. Because, the rotational path of 2 around 1 can be moved out of the 2D plane on which particles 1+2 reside. Then we can adiabatically contract the path to vanish. Therefore, 3D a simply connected space. So, the wavefunction must come to itself after 2π rotation (single-valued wavefunction). In other words P^2 should give the same wave function, ie, its an eigenstate of P^2 with eigenvalue 1:

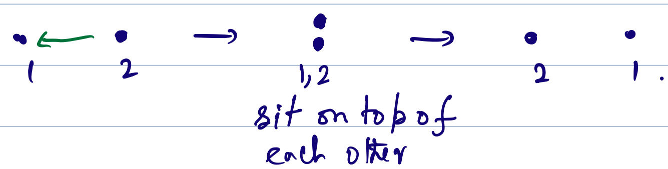
$$P^2 \psi(1,2) = \psi(1,2)$$

$$\text{or,} \quad e^{2\theta} = 1 \Rightarrow \theta = 0 \quad \text{bosons}$$

$$\text{or} \quad = \pi \quad \text{fermions}.$$

Therefore, in 3D and higher dimensions only boson and fermion particles are possibles, where as in 2D one can have more exotic particles, called anyons.

<u>1D:</u> 1D is tricky. Here the exchange between two particles



require the two particles to sit on top of each other, ie, they occupy the same state in the intermediate step. Here this becomes impossible to distinguish between a statistical exchange and interaction. If the wavefunction changes sign when two particles swap their positions, one can say either they are fermions or interacting bosons which allowed two particles to pass through each other and the interaction generated a π-phase. This concept is in the root of the Bosonization technique for describing interacting fermions in 1D in terms of bosons or vice versa.

Many-body wave function for identical particles:

$$\left.\begin{aligned} \text{Bosons:} \quad & \psi(r_1, r_2, \cdots, r_N) = \psi(\vec{r}_2, \vec{r}_1, \cdots, \vec{r}_N). \\ \text{Fermions:} \quad & \psi(\vec{r}_1, \vec{r}_2, \cdots, r_N) = -\psi(\vec{r}_2, \vec{r}_1, \cdots, \vec{r}_N). \end{aligned}\right\} \quad (4)$$

$$= (-1)^p \psi(\vec{r}_p, \vec{r}_2, \cdots \vec{r}_1, \cdots, r_N).$$

where p is the number of exchanges or permutations require to bring the wave function in the same ordering as on the left hand side.

$$\text{Anyons (2D):} \quad \psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N) = \left(e^{i\theta}\right)^p \psi(\vec{r}_p, \vec{r}_2, \cdots, \vec{r}_1, \cdots \vec{r}_N).$$

- If we have a N-site lattice and at each site, we have a single electronic state; ei, 2 states per site. Then the total number of states is $2^N = e^{N \ln 2}$. This is an exponentially large number of states and it becomes impossible to solve the problem analytically or numerically.

- The first set of approximation is to take a product state of single particle states $u_\alpha(r_i)$, vary them in the variation approach. This brings down the Hilbert space dimension to N. But the particles are identical, so we have many permutations of states and particles that are possible. Although such permuted states are linearly independent to each other, they form a vector space and we have to consider their linear combinations. Then we have to be careful about how each permutation is related to each other, as there is sign change for each mutual exchange. Therefore, we can express the product state in eq(4) more appropriately for identical particles as follows.

For fermions:

$$\psi_{\alpha_1 \cdots \alpha_N}(r_1 \cdots r_N) = \frac{1}{\sqrt{N!}} \sum_P (-1)^P P\, u_{\alpha_1}(r_{P_1})\, u_{\alpha_2}(r_{P_2}) \cdots u_{\alpha_N}(r_{P_N})$$

(This is just a Slater determinant) $\cdots$ (5a)

For bosons.

$$\psi_{\alpha_1 \cdots \alpha_N}(r_1 \cdots r_N) = \frac{1}{\sqrt{N_+}} \sum_P P\, u_{\alpha_1}(r_{P_1})\, u_{\alpha_2}(r_{P_2}) \cdots u_{\alpha_N}(r_{P_N}) \quad \cdots (5b)$$

where P stands for permutation, r_{P_1} is the particle r in the pth permutation.

- The normalization factor for fermions is $\frac{1}{\sqrt{N!}}$. This is easy to fix. Because, here we have $N!$ ways to choose a given permutation. Then in the inner product $\langle \psi_{\alpha_1 \cdots \alpha_N}(r_1 \cdots r_N) | \psi_{\alpha_1 \cdots \alpha_N}(r_1 \cdots r_N) \rangle$, for a given permutation on the ket state, there is only one permutation on the bra state that contributes. Cause, each permutation is linearly independent. Since we have $N!$ permutation, so, $\langle \psi | \psi \rangle = N!$ and the P sum runs over $N!$ values.
- The normalization for boson is tricky, since one can have multiple particles on the same state u_α. We still have $N!$ ways to chose a given configuration with one particle per site. The second configuration is one state has two particles and others have one particle, and one state has no particle. Such a configuration also have $N!$ permutations. This way we obtain $N_+ = N! \prod_i n_{\alpha_i}!$, where $\sum_i n_{\alpha_i} = N$.

- Therefore, fermionic state can alternatively be written as Slater determinant state. The bosonic state is called the "permanent" state. The renormalization factors help reduce the number of basis states from 2^N states due to permutation symmetry.

- Product states have no correlation between each particles. But the above quantum states - which are the linear superposition of many possible product states has in-built correlation between the particles. This plays important roles in the quantum phase transitions.

→ The Shortcomings of First quantization :

There are a couple of shortcomings of the 1st quantization method. (I) Because here the number of particles are fixed, so this theory cannot describe the system where particles are created or annihilated, i.e. systems where particle number is not conserved. Again in many-body variational approach, we first obtain the ground state and then a few excited state. In such approach first quantization will be very difficult since here one solves for the full Hilbert space. Each time we change N, we have a new Hilbert space, i.e. a new system. (II) Since particles are identical, its too much redundant to study each particles and find out in which state it goes to.

Second Quantization:

The second quantization uses operator to define states and the exchange symmetry is converted into commutation relation between the operators. Here we change the perspective. Instead of looking at the coordinates of all particles $(r_1, r_2, \ldots, r_N)$, we now consider a state of occupation $(n_{\alpha_1}, n_{\alpha_2}, \ldots, n_{\alpha_N})$, and ask whether the state is empty or occupied. We don't care about which particle occupies the state, because they are all identical. So, to define a state, we just need to give the occupation numbers in all the states.

The state is fixed, taken as the Hilbert space of a fixed operator which has nothing to do with the Hamiltonian. The most common operator is the number operator as we have learned in the Harmonic oscillator case. We then have to express the Hamiltonian in this Hilbert space.

This procedure makes our life much easier, since now we do not have to worry about which particle we are inserting. Because they are all identical. The symmetry and anti-symmetry properties of the wavefunction in the first quantization case which was associated with identical particles, get converted to how many particles a state can occupy, and the commutation/anti-commutation relation of the particle creation/annihilation operators. For bosons, we have infinite occupancy in a state. Hence, its an infinite dimensional Hilbert space and the number of particles is not conserved. For fermions, its single particle per state, and one has a two dimensional Hilbert space at each site (empty or singly occupied).

What we have done, mathematically, is that we have inserted a Harmonic oscillator (H.O.) for each state for bosons. (We will first focus on bosons, and for fermions, its actually a two-dimensional harmonic oscillator - something that is abstract or formal). Note that we have inserted an H.O. for each basis state $\psi_{k,n}$, not for each eigenvalue $E_n(k)$, because one can have degeneracy for a eigenvalue. So, we have to insert an H.O. for each basis state. This approach is applicable even when the number operator $\hat{N}$ does NOT commute with the Hamiltonian.

This can also be perceived as filling each basis state one by one. But since at each state, we have an infinite dimensional Hilbert space, ie, one can fill each state by infinite number of particles, so the 2nd quantized Hilbert space does not conserve particle number N. For any values of N, we have the same Hilbert space. A given value of N corresponds to a particular 1st quantized system, which is a subsystem of the infinite dimensional Hilbert space. This is sometimes called the Fock space. Another system with a different number of particle is another subsystem of the same Fock space. Each particle carry a quanta of energy e_α in the basis state $\psi_{i,\alpha}$ is the eigenstate of $h(\vec{r}_i)$. This is same as a H.O. with frequency $\omega_\alpha = e_\alpha/\hbar$ is added to the system, which increases the energy of the system by $\hbar\omega_\alpha = e_\alpha$.

The Fock space or the many-body state in 2nd quantization is denoted by a state vector

$$|n_{\alpha_1}\, n_{\alpha_2} \cdots \rangle = |n_{\alpha_1}\rangle \otimes |n_{\alpha_2}\rangle \otimes \cdots \qquad \cdots (1)$$

where $\alpha_1, \alpha_2, \cdots$ refer to the basis state, and n_{α_i} are their occupation numbers.

For systems of fixed number of particle, one has the constraint

$$\sum_i n_{\alpha_i} = N.$$

For bosons: $n_{\alpha_i} = 0, 1, 2, \cdots \infty$.

For fermions: $n_{\alpha_i} = 0, 1$.

- Next we introduce some abstract/formal creation and annihilation operators of particles in the state $|\alpha\rangle$ as $a_\alpha^\dagger$, a_α, respectively. These are like the ladder operators we encountered in the case of H.O., which takes us from one state to another with different particle numbers. (In the case of H.O., these operators are constructed from the position & momentum operators $\hat{p} \pm i\hat{x}$. However, in the 2nd quantization, one should not think of them to necessarily arise from such physical operators even for the bosonic case. We should just treat them as abstract operators).

- Next we introduce the concept of a vacuum state $|0\rangle$ with no particle, which is destroyed by a_α

$$a_\alpha |0\rangle = 0 \qquad \cdots (2a).$$

Then a single particle state is $|1\rangle = a_\alpha^+|0\rangle$ (we did not insert the index 'α' in the state for simplicity in notation).

The n_{α_i}-particle state at the α_i-site:

$$|n_{\alpha_i}\rangle = \frac{1}{\sqrt{n_{\alpha_i}!}}\left(a_{\alpha_i}^+\right)^{n_{\alpha_i}}|0\rangle \quad \text{--- (2b)}$$

This way, we define the N-particle many-body state as

$$|n_{\alpha_1}, n_{\alpha_2} \cdots\rangle = \frac{1}{\sqrt{\underbrace{N! \prod_i n_{\alpha_i}!}_{N_+}}}(a_{\alpha_1}^+)^{n_{\alpha_1}}(a_{\alpha_2}^+)^{n_{\alpha_2}} \cdots \underbrace{|0\,0\cdots\rangle}$$

Often simply denoted by $|0\rangle$.

with the constraint $\sum_i n_{\alpha_i} = N$. --- (2c).

First Quantization — Second Quantization

$$\rightarrow \phi_{\alpha_1,\alpha_2,\cdots,\alpha_N}(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_N) \longleftrightarrow |n_{\alpha_1}, n_{\alpha_2}\cdots\rangle = \frac{1}{\sqrt{N_+}}(a_{\alpha_1}^+)^{n_{\alpha_1}}(a_{\alpha_2}^+)^{n_{\alpha_2}}\cdots|0\rangle$$

The claim is that the 1st quantized state, which is symmetrized/anti-symmetrized for bosons/fermions corresponds to a Fock state in the 2nd quantization which is properly ordered including normalization. The ordering of the operators $a_{\alpha_1}^+, a_{\alpha_2}^+ \cdots$ takes care of the symmetry/anti-symmetry property. This means, if we exchange $a_{\alpha_1}^+ a_{\alpha_2}^+ \rightarrow a_{\alpha_2}^+ a_{\alpha_1}^+$, nothing happens if they are bosons or obtain a negative sign if they are fermions. This means $a_{\alpha_i}^+$ commute or anticommute for bosons or fermions. For bosons,

$$[a_\alpha, a_\beta^+] = \delta_{\alpha\beta}, \quad [a_\alpha, a_\beta] = 0, \quad [a_\alpha^+, a_\beta^+] = 0.$$

This commutation relations are crucial to the statistics of the particle and must remain invariant under a unitary transformation. The unitary transformation that preserves the commutation relation of particles is called the cannonical transformation. Fourier transformation is a canonical transformation and hence commutation relations hold both for the real space site indices as well as in the momentum space.

- The ladder operation is similar to the H.O. case $a^{\dagger}|n\rangle = \sqrt{n+1}\,|n+1\rangle$ and $a|n\rangle = \sqrt{n}\,|n-1\rangle, \forall \alpha$.

- Although we will discuss the operator formulation in the second quantization, its worth looking at the Hamiltonian and number operator here.

  The Hamiltonian in first and 2nd quantizations are not the same, but the mapping between them are exact.

First quantization. Second Quantization

$$H \psi_{\alpha_1, \cdots \alpha_N}(r_1, \cdots r_N) = \left(\sum_{\alpha=1}^{N} e_\alpha\right) \psi_{\alpha_1 \cdots \alpha_N}(r_1 \cdots r_N) \longrightarrow H|n_{\alpha_1}, n_{\alpha_2} \cdots\rangle = \left[\sum_i \hbar \omega_{\alpha_i}(a^{\dagger}_{\alpha_i} a_{\alpha_i} + 1)\right] |n_{\alpha_1}, n_{\alpha_2} \cdots\rangle.$$

where $h_\alpha \psi_\alpha(r_\alpha) = e_\alpha \psi_\alpha(r_\alpha)$ for single particles.

+ zero point (constant) vacum energy --(3)

These two Hamiltonians are exact mapping to each other when $e_\alpha = \hbar \omega_\alpha$. So, each eigenstate is an oscillator, like photon, phonon.

- The information about the number of particle is embedded in the eigenvalue of the number operator $\hat{N} = \sum_{\alpha=1}^{\infty} a^{\dagger}_\alpha a_\alpha$.

$$\hat{N}\,|n_{\alpha_1} n_{\alpha_2}\cdots\rangle = \hat{N}\,(a^+_{\alpha_1})^{n_{\alpha_1}}(a^+_{\alpha_2})^{n_{\alpha_2}}\cdots\,|n_{\alpha_1} n_{\alpha_2}\cdots\rangle$$

$$= \underset{\uparrow}{N}\,|n_{\alpha_1} n_{\alpha_2}\cdots\rangle \qquad \text{--- (4)}$$

eigenvalue of $\hat{N}$

where we have used the commutation relations $[N, \hat{a}_\alpha] = a^+_\alpha$, $[N, a^+_\alpha] = -a_\beta$. In the above we have also assumed $[\hat{N}, \hat{H}] = 0$, which is not necessarily the case always.

- **Fermions:** Here we really don't have a physical harmonic oscillator at each basis state. We have to introduce the fermion creation operator c^+ by hand in analogy with the bosonic oscillator case. We denote c^+, c for fermion case as often done in the literature. We introduce an 2D Hilbert space at each basis state (i.e. at each site) in an abstract/formal way, on which a set of creation & annihilation operators are defined as c^+_α & c_α, which satisfy:

$$\{c_\alpha, c_\beta\} = \{c^+_\alpha, c^+_\beta\} = 0 \qquad \text{--- (5a)}$$

$$\{c_\alpha, c^+_\beta\} = \delta_{\alpha\beta} \qquad \text{--- (5b)}$$

where $\{\ \}$ stands for anticommutation relation.

→ There are two important properties that become obvious from this anti-commutation algebra:

(i) $c^+_\alpha c^+_\beta = -c^+_\beta c^+_\alpha$, which means as we exchange two fermions we 'n a '−' sign. This is consistent with asymmetric statistics of fermions.

(ii) $c^+_\alpha c^+_\alpha = -c^+_\alpha c^+_\alpha = 0$, for $\alpha = \beta$. This means, at a given state, two or more fermions can not occupy – Pauli Exclusion Principle.

→ At a given basis / eigen state, we have two fermionic Fock states $|0\rangle$ & $|1\rangle$, i.e, we insert a 2D Fock space for fermions. $|0\rangle$ is the vacuum state defined similarly by a state that is annihilated by 'c' as $c\,|0\rangle = 0$.

Then $\quad |1\rangle = c^{+}|0\rangle, \quad c|1\rangle = |0\rangle, \quad c^{+}|1\rangle = 0. \quad$ --- (6)

and $\quad (c^{+})^{2}|0\rangle = 0$, as $c^{+2} = 0$ due to its anticommutation property.

→ We will introduce a 2nd quantized Hamiltonian, which has a one-to-one mapping to the original non-interacting Hamiltonian as

$$\hat{H} = \sum_{\alpha=1}^{\infty} e_{\alpha}\, c_{\alpha}^{+} c_{\alpha} \qquad \text{--- (7)}$$

→ We can also show that each many-body state in the 2nd quantization corresponds uniquely to that in the 1st quantization with the same energy, i.e.

$$\Psi_{\alpha_1 \cdots \alpha_N}(r_1 \cdots r_N) \longleftrightarrow c_{\alpha_1}^{+} c_{\alpha_2}^{+} \cdots c_{\alpha_N}^{+} |0\rangle,$$

upto some normalization.

Here, however, we have to be careful for fermions about the ordering of the operators $c_{\alpha_1}^{+}, c_{\alpha_2}^{+} \cdots$. This was not a problem for bosons since they commute. But for fermions it matters since they anticommute – which corresponds to the antisymmetric wave function in 1st quantization. We usually choose some convention – leading to normal ordering. For example, we order them in increasing in energy eigenvalues or momentum or from lattice sites starting from the left hand side, etc. Once we choose a convention, we then stick to it.

Lets say we start with a convention as $|n_1 n_2 \cdots n_\alpha \cdots\rangle$, where $n_\alpha = 0, 1$. Then we apply an annihilation operator c_α to destroy a particle on the α^{th} state

$$c_\alpha |n_1 n_2 \cdots n_\alpha \cdots\rangle = c_\alpha c_1^\dagger c_2^\dagger \cdots c_\alpha^\dagger \cdots |0\rangle \quad \text{--- (8a)}$$

$$= (-1)^{\sum_{i=1}^{\alpha-1} n_i} \sqrt{n_\alpha}\, |n_1 n_2 \cdots n_\alpha - 1 \cdots\rangle \quad \text{--- (8b)}$$

→ If $n_\alpha = 0$, i.e., if n_α state is empty, then R.H.S is zero as expected from eq(5).

→ The phase factor $(-1)^{\sum_{i=1}^{\alpha-1} n_i}$ is important for fermions. Because we have to skip $\alpha-1$ previous states before reaching the α^{th} state. This phase factor is called the Fermion parity. As all the states and their corresponding operators are ordered in increasing number, by convention, to bring the c_α operator to the α^{th} position, it has to anti commute with all the previous $a_i^\dagger$ operators upto $\alpha-1$. Then each anticommutation yields a '-1' phase and the total phase is $(-1)^{\sum_{i=1}^{\alpha-1} n_i}$.

→ Similarly, $c_\alpha^\dagger |n_1 \cdots n_\alpha \cdots\rangle = (-1)^{\sum_{i=1}^{\alpha-1} n_i} \sqrt{1-n_\alpha}\, |n_1 \cdots n_\alpha + 1 \cdots\rangle$.
— (9).

- Anyons: We can generalize these notations to anyons, which get a statistical phase of $0 \le \theta \le \pi$ each time two anyons are exchanged. $\theta = 0, \pi$ for bosons & fermions, respectively.

→ Graded commutation relations:

$$\left.\begin{aligned} a_\alpha a_\beta - e^{i\theta} a_\beta a_\alpha &= 0. \\ a_\alpha^\dagger a_\beta^\dagger - e^{i\theta} a_\beta^\dagger a_\alpha^\dagger &= 0 \\ a_\alpha a_\beta^\dagger - e^{i\theta} a_\beta^\dagger a_\alpha &= \delta_{\alpha\beta}. \end{aligned}\right\} \quad \text{— 10}$$

→ $$a_\alpha |n_1 \cdots n_\alpha \cdots\rangle = \left(e^{i\theta}\right)^{\sum_{i=1}^{\alpha-1} n_i} \sqrt{n_\alpha}\, |n_1 \cdots n_{\alpha-1} \cdots\rangle$$

$$a_\alpha^\dagger |n_1 \cdots n_\alpha \cdots\rangle = \left(e^{i\theta}\right)^{\sum_{i=1}^{\alpha} n_i} \sqrt{1+e^{i\theta} n_\alpha}\, |n_1 \cdots n_\alpha + 1 \cdots\rangle.$$

(There are clearly some inconsistency for anyons, suggesting that the Fock space formalism does not quite work for anyons, other than $\theta = 0, 1$.)

Operators in Second Quantization

So far we have talked about state vectors in two different quantization languages. What are the good / allowed operators ? Ans: Those which are Hermitian and symmetric under particle exchange / permutation are allowed operators. e.g. $\hat{x}_i$, $\hat{p}_i$ for a single particles in many body systems are not good operators, since for identical particles, it does not make sense to consider a single particle operator.

A good operator is that does not distinguish between different particles, i.e., the operator must commute with the permutation operator P. A good operator is then $\sum_{i=1}^{N} x_i$ or $\sum_{i}^{N} p_i$, i.e., total position, total momentum of the system, as these operators are symmetric under the exchange of particles.

⊛ Let us first review the operator formalism in first quantization case.

→ **One Body Operator:**

The single particle operator in the many-body setting is generally defined to be

$$\hat{V} = \sum_{i=1}^{N} \hat{v}(r_i) \quad \cdots (11)$$

Examples of single particle operators are : $v(r_i) \equiv x_i, p_i, x_i p_i,$ ∇_i, ∇_i^2, and so on.

Then we want to compute the matrix element of this operator with respect to the wavefunction in eq (5a) or (5b) as

$$\langle \psi | V | \psi \rangle = \int dr_1 \cdots dr_N \, \psi^*(r_1, \cdots, r_N) \sum_{i=1}^{N} v(r_i) \, \psi(r_1, \cdots r_N) \quad \text{--- (12)}$$

There are too many terms, $\sim N!$ due to permutation in the wavefunction as well as N-terms in V. But since the single particle states are orthogonal to each other, there is only one term that will contribute for the operator at $v(r_i)$, and that is $u^*_\alpha(r_i), u_\alpha(r_i)$, while $u^*_\alpha(r_j) \, u_\alpha(r_j)$ terms for $j \neq i$ are all normalized to 1. For bosons, there is however an additional criterion that a given state can be occupied by multiple particles, which is denoted by the occupation number n_i of this state. So we get

$$\langle \psi | V | \psi \rangle = \sum_\alpha n_\alpha v_{\alpha\alpha}, \text{ where } v_{\alpha\alpha} = \int d^3r \, u^*_\alpha(r) \, v(r) \, u_\alpha(r).$$
$$= \langle n_1 \cdots n_\alpha \cdots | V | n_1 \cdots n_\alpha \cdots \rangle \quad \text{--- (13)}$$

[This is generally lengthy to derive and one can try it for 2 or 3 particles. The 'n_α' term arises for boson can be shown to arise from the fact that a given state α can be filled by n_α number of particles.

- In the above case we have assumed that $v(\vec{r}_i)$ commutes with $h(r_i)$, so that $u_\alpha(r_i)$ are the eigen states of $v(r_i)$ as well. In general, this is not necessarily true. Then $v(r_i)$ will be a matrix in the $u_\alpha(r_i)$ basis, and the diagonal terms are given by eq (13), and the off-diagonal terms ($v_{\alpha\beta}$) are expressed as:

$$\langle n_1 \cdots n_\alpha + 1 \cdots n_\beta - 1 \cdots | V | n_1 \cdots n_\alpha \cdots n_\beta \cdots \rangle$$

$$= \sqrt{(n_\alpha+1)\, n_\beta}\;\; v_{\alpha\beta} \;,\;\; v_{\alpha\beta} = \int d^3r\, u_\alpha^*(r)\, v(r)\, u_\beta(r) \quad (14a)$$

for bosons ---

$$= (-1)^{\sum_{\alpha<i<\beta} n_i} \sqrt{(n_\alpha+1)\, n_\beta}\;\; v_{\alpha\beta} \quad \text{for fermions.} \quad ---(14b)$$

- The origin of the pre-factor $\sqrt{(n_\alpha+1)\, n_\beta}$ in 1st quantization is rooted in the normalization factor of $1/\sqrt{N!\prod_\alpha n_\alpha}$, which makes the numerator $\sqrt{n_\beta}$ for n_β occupied ket state.
- This is like the operator takes a particle from β-state and insert it in the α-state. Clearly $n_\beta \neq 0$ for this scattering/tunneling to take place. For fermions, n_α also has to be empty for this case. For fermions, the additial phase factor comes due to antisymmetrization of the single particle states in going from α to β-states.

→ Two body operator: $W = \frac{1}{2}\sum_{i\neq j} w(r_i, r_j)$

(The factor of ½ is to avoid double counting). This is a symmetric operator as $w(r_i, r_j) = w(r_j, r_i)$, and more often $w(|\vec{r}_i - \vec{r}_j|)$ is a function of the relative distance.

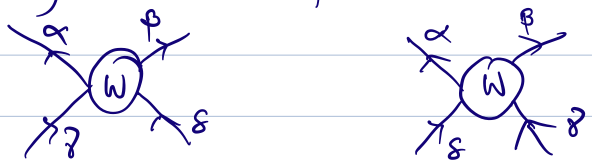
The matrix elements of W are non-zero when two-particles change states, ie, this potential can move two particles out of two states or same state (if bosons). Lets say w-potential moves two particles from state γ, δ to α, β. So, it decreases n_γ to $n_\gamma - 1$, $n_\delta \to n_\delta - 1$ and increases n_α to $n_\alpha + 1$, n_β to $n_\beta + 1$. So, we get

$$\langle \cdots n_\alpha+1 \cdots n_\beta+1 \cdots n_\gamma-1 \cdots n_\delta-1 \cdots | W | \cdots n_\alpha \cdots n_\beta \cdots n_\gamma \cdots n_\delta \cdots \rangle$$
$$= \frac{1}{2}\sqrt{(n_\alpha+1)(n_\beta+1)\, n_\gamma\, n_\delta} \times (\text{Phase factor for fermions})$$
$$\times \Big(\underbrace{\langle \alpha\beta | w | \gamma\delta \rangle}_{w_{\alpha\beta\gamma\delta}} + \gamma \underbrace{\langle \alpha\beta | w | \delta\gamma \rangle}_{w_{\alpha\beta\delta\gamma}} \Big) \quad -(15)$$

where $W_{\alpha\beta\gamma\delta} = \langle \alpha\beta | W | \gamma\delta \rangle = \int d^3r\, d^3r'\; u_\alpha^*(r)\, u_\beta^*(r')\, W(r,r')\, u_\gamma(r)\, u_\delta(r')$

& $W_{\alpha\beta\delta\gamma} = \langle \alpha\beta | W | \delta\gamma \rangle = \int d^3r\, d^3r'\; u_\alpha^*(r)\, u_\beta^*(r')\, W(r,r')\, u_\delta(r)\, u_\gamma(r')$.

which correspond to the two possibilities of $\gamma \to \alpha,\ \delta \to \beta$ & $\delta \to \alpha,\ \delta \to \beta$.



These two terms are related to each other by a fermion phase factor of $\zeta = -1$. The ordering of the states is important for fermions because of the fermion parity.

H.W. Work out the phase factor in eq (15).

Operators in Second Quantization

Now its easy to express the two operators in the second quantization formula, where $n_\alpha \to \hat{a}_\alpha^\dagger \hat{a}_\alpha$.

Proof: $\hat{V} = \sum_{i=1}^{N} v(r_i) \longrightarrow \hat{V} = \sum_{\alpha,\beta=1}^{N} v_{\alpha\beta}\, a_\alpha^\dagger a_\beta \quad \cdots (16)$

where $v_{\alpha\beta} = \int d^3r\; u_\alpha^*(r)\, v(r)\, u_\beta(r)$.

In the first quantization, the one body operator gives a transition from state β to α. In the 2nd quantization, this is equivalent to destroying a particle in the β-state and creating a particle at the α-state. $v_{\alpha\beta}$ is the energy cost for this transition/scattering.

[Here we have to prove that

$$\langle V\rangle = \langle 0|\, a_{n_1} \cdots a_{n_\alpha} \cdots a_{n_\beta} \cdots a_{n_N} \Big| \sum_{\alpha=1}^{N} v(r_i) \Big|\, a^+_{n_1} \cdots a^+_{n_\alpha} \cdots a^+_{n_\beta} \cdots a^+_{n_N} |0\rangle$$]

- Similarly, the two body operator is written as

$$\hat{W} = \sum_{\alpha\beta\gamma\delta=1}^{\infty} W_{\alpha\beta\gamma\delta}\, a^+_\alpha a^+_\beta a_\delta a_\gamma. \quad --- \quad (17),$$

where $W_{\alpha\beta\gamma\delta}$ is same as before.

- It is customary to write all the creation operators on the left and annihilation operators on the right. The ordering among the creation operator is up to the convention one choses.
- Notice that the ordering among $\alpha\beta\gamma\delta$ in W and those in a^+, a are different. This comes from the ordering of the derivation

- In the 1st quantization, we had a summation over N-dim Hilbert space. But in 2nd quantization, the summations is extended to infinity. The $n_\alpha = 0$ value for states above the N-dim Hilbert space takes care of it.

  So, in the 2nd quantization, there is no explicit N-dependence. It's analogous to the cannonical and grand cannonical ensemble cases for 1st and 2nd quantization cases.

- All operators defined in 1st quantization is also defined in the 2nd quantization. But in second quantization, we can define more operators that do not conserve particle number, such as a^+a^+, aa, etc, which are non-Hermitian.

- Hamiltonian:

1st Quantization → 2nd Quantization

$$\hat{H}_N = \sum_{i=1}^{N} h_i + \sum_{i\neq j}^{N} v_{ij} \longrightarrow \hat{H} = \sum_{\alpha,\beta}^{\infty} \varepsilon_{\alpha\beta}\, c_\alpha^+ c_\beta + \sum_{\alpha\beta\delta\gamma} v_{\alpha\beta\delta\gamma}\, c_\alpha^+ c_\beta^+ c_\gamma c_\delta$$

$\alpha, \beta, \gamma, \delta$ can be site indices in the real space Hamiltonian or can be 'k' in the momentum space. ... (18)

here $\varepsilon_{\alpha\beta} = \langle\alpha| T_e + V_{eI} |\beta\rangle$, which is the non-interacting Hamiltonian

$$v_{\alpha\beta\delta\gamma} = \langle\alpha|\langle\beta| \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} |\gamma\rangle|\delta\rangle.$$

H.W. Do a Fourier transformation of the creation and annihilation operators to express the many-body electron Hamiltonian in the momentum space. In the momentum space, the first term should be diagonal.

Basis Transformation, Fourier Transformation

An important feature to remember for the creation & destruction operators in that, despite we call them operators, they transform like a state under any unitary transformation. This is also obvious because they actually represent states, ie, they act on some vacuum state and give a new state. We can see that as follows. Lets say $|\alpha\rangle \in \mathcal{H}$ is some state in the Hilbert space $\mathcal{H}$, and we transform it to $|n\rangle$ which are related to $|\alpha\rangle$ states by some unitary transformation U as

$$|n\rangle = \sum_\alpha U_{n\alpha} |\alpha\rangle = \sum_\alpha \langle\alpha|n\rangle |\alpha\rangle .$$

Now, lets define $a_n^\dagger$ & $a_\alpha^\dagger$ being the creation operators in the $|n\rangle$ & $|\alpha\rangle$ states as $|n\rangle = a_n^\dagger|0\rangle$, $|\alpha\rangle = a_\alpha^\dagger|0\rangle$. The vacuum $|0\rangle$ remains unchanged in both space. Then we obtain

$$a_n^\dagger = \sum_\alpha U_{n\alpha} a_\alpha^\dagger .$$

The unitary transformation is a canonical transformation, under which the commutation relation among $a_n^\dagger, a_m^\dagger$ remain same to the commutation relation between $a_\alpha^\dagger, a_\beta^\dagger$.

Fourier transformation is a special type of cannonical transformation from real space $(\alpha \equiv i)$ to momentum space $(n \equiv k)$, where the basis functions are $\langle i | k \rangle = \frac{1}{\sqrt{V}} e^{-i\vec{k}\cdot\vec{r}_i}$

Then we write the ladder operators in the fourier space as

$$a_k^+ = \frac{1}{\sqrt{V}} \sum_i e^{-i\vec{k}\cdot\vec{r}_i} a_i^+$$

and $$a_i^+ = \frac{1}{\sqrt{V}} \sum_k e^{i\vec{k}\cdot\vec{r}_i} a_k^+ .$$

Field operators: Creation/annihilation operators in position space.

We introduce the creation and destruction operators in some single particle state α as a_α, $a_\alpha^\dagger$. Now, we want to obtain such creation & annihilation operator in some other state. One would then simply do a basis transformation in the usual way, making sure the commutation/anti-commutation relation among the creation & annihilation operators remain the same, because otherwise the fermionic/bosonic properties of the particle will change, which is not allowed. The basis transformation that follows this property is called the cannonical transformation.

A particular type of such transformation in which one defines creation and annihilation operators in the <u>continuous position</u> $\vec{r}$ from the collection of states α gives us Field operators:

$$\underbrace{\hat{\psi}_\sigma}_{\text{operator}}(\vec{r}) = \sum_\alpha \underbrace{\phi_{\alpha,\sigma}}_{\text{function}}(\vec{r})\ \underbrace{\hat{a}_{\alpha,\sigma}}_{\text{operator}} \quad \cdots \quad (19a)$$

where $\phi_{\alpha,\sigma}(\vec{r})$ are the complex wavefunction of the state α in the position space. We introduce another quantum number 'σ' in the position space, which is like spin/orbital etc.

The inverse transformation is

$$\hat{a}_{\alpha,\sigma} = \int d^3r\ \phi^*_{\alpha,\sigma}(\vec{r})\ \hat{\psi}_\sigma(\vec{r}) , \quad \cdots \quad (20a)$$

This is actually a transformation from α-states to the position states. The transformation is possible if $\phi_{\alpha,\sigma}(\vec{r})$ are orthonormalized, which is provided.

• Example: Assume $\alpha = \vec{k}$, momentum states. Then eq (19) is like a fourier transformation from the momentum state to the position states, and the wave functions $\phi_{k\sigma}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$. Therefore, we rewrite eq (19) + (20) as

$$\hat{\psi}_\sigma(\vec{r}) \equiv \hat{a}_\sigma(\vec{r}) \equiv \frac{1}{\sqrt{V}} \sum_k e^{i\vec{k}\cdot\vec{r}} \hat{a}_{k\sigma} \quad \text{--(19b)}$$

(Sometimes the field operators are denoted by the same variable $\hat{a}_n(\vec{r})$ or $\hat{a}_{n,r}$ for simplicity)

And, $$\hat{a}_{k\sigma} = \frac{1}{\sqrt{V}} \int d^3r \, e^{-i\vec{k}\cdot\vec{r}} \hat{a}_\sigma(\vec{r}) \quad \text{--(20b)}$$

• H.W. Show that
$$\{\hat{a}_\sigma(\vec{r}), \hat{a}^+_{\sigma'}(\vec{r}')\} = \delta^{(3)}(\vec{r}-\vec{r}')\,\delta_{\sigma,\sigma'}$$
$$\{\hat{a}_\sigma(\vec{r}), \hat{a}_{\sigma'}(\vec{r}')\} = \{\hat{a}^+_\sigma(\vec{r}), \hat{a}^+_{\sigma'}(\vec{r}')\} = 0. \quad \text{--(21)}$$
provided $\hat{a}_{k\sigma}$ also follow the same anticommunation algebra. and similar for bosons with commutation relation.

• The number density operator is

$$n_\sigma(\vec{r}) = \sum_i \delta(\vec{r} - \vec{r}_{i,\sigma})$$, where $\vec{r}_{i,\sigma}$ is the position of the i^{th} particle of σ-spin in 1st quantization

$\because \delta(r - r_i) = \sum_k e^{i\vec{k}\cdot(\vec{r}-\vec{r}_i)}$ & $|k,\sigma\rangle = a^+_{k\sigma}|0\rangle$

$$= \sum_i \sum_{k,k',k''} |k',\sigma\rangle \underbrace{\langle k',\sigma| e^{i\vec{k}\cdot(\vec{r}-\vec{r}_i)} |k'',\sigma\rangle}_{\delta_{k,k''-k'}} \langle k'',\sigma|$$

$$= \sum_i \sum_{k',k''} \underbrace{e^{-i\vec{k}'\cdot(\vec{r}-\vec{r}_i)} a^+_{k'\sigma}}_{\psi^+_\sigma(r)} \underbrace{e^{i\vec{k}''\cdot(\vec{r}-\vec{r}_i)} a_{k'',\sigma}}_{\psi_\sigma(r)} |0\rangle\langle 0|$$

from eq 19b.

$$= \hat{\psi}^+_\sigma(\vec{r})\,\hat{\psi}_\sigma(\vec{r}). \quad \text{--(22)}$$

- Show that the density operator in the momentum space is $\hat{n}_{k,\sigma} = \sum_i e^{-ik\cdot\vec{r}_{i,\sigma}}$ in the 1st quantized notation & $\hat{n}_{k,\sigma} = a^+_{k\sigma} a_{k\sigma}$ in 2nd quantization.

- Total number of particles $\hat{N}_\sigma = \int d^3r \; \psi^+_\sigma(\vec{r}) \psi_\sigma(\vec{r})$
$$= \sum_k a^+_{k\sigma} a_{k\sigma}.$$

- These density operators are extremely useful operators in condensed matter. One can further change the way of solving the problem from single particle states/coordinates $\vec{r}_i$ to general position space. Instead of looking at each particles' coordinates $\vec{r}_i$, we now sit at a position $\vec{r}$ and ask how many particles are present at that position at a time, i.e., the density. This is analogous to the ensemble theory in going from microscopic Newtonian mechanics to statistical physics. This field operator definition is at the heart of the Quantum Field Theory, as well as the Density Functional Theory.

We write the operators in terms of density operators as follows:

$$V = \sum_i v(\vec{r}_i)$$

$$= \int d^3\vec{r} \; v(\vec{r}) \underbrace{\sum_i \delta(\vec{r}-\vec{r}_i)}_{\psi^+(\vec{r})\psi(\vec{r})} \quad \text{in 1st quantization}$$

from eq (22)

$$= \int d^3\vec{r} \; v(\vec{r}) \underbrace{\psi^+(\vec{r}) \psi(\vec{r})}_{n(\vec{r})}. \quad \text{in Field operator form.} \qquad \text{--- (23a)}$$

Now, we can write it in any basis: α, β or k basis as follows:

$$= \sum_{\alpha,\beta} \underbrace{\langle \alpha | v | \beta \rangle}_{v_{\alpha\beta}} a_\alpha^+ a_\beta \quad \text{in 2nd quantization}$$

$$v_{\alpha\beta} = \int d^3r\, u_\alpha^*(r)\, v(\vec{r})\, u_\beta(\vec{r}).$$

$$= \sum_k v_{k,k}\, a_k^+ a_k \,, \quad \text{in momentum space,} \qquad \text{--- (23b)}$$

where its diagonal due to translational invariance.

Similarly, the two body operator is

$$W = \frac{1}{2} \sum_{i \neq j} w(\vec{r}_i, \vec{r}_j)$$

$$= \frac{1}{2} \sum_{i,j} W(\vec{r}_i, \vec{r}_j) - \frac{1}{2} \sum_{i=i} w(\vec{r}_i, \vec{r}_i)$$

, we remove the $i \neq j$ condition, then subtract the diagonal term.

Now, we can write it in terms of the density operator $\hat{n}(\vec{r})$ as

$$= \frac{1}{2} \int d^3\vec{r}\, d^3\vec{r}\,'\, W(\vec{r}, \vec{r}\,')\, n(\vec{r})\, n(\vec{r}\,') - \frac{1}{2} \int d^3r\, W(\vec{r}, \vec{r})\, n(\vec{r}).$$

$$= \frac{1}{2} \int d^3\vec{r}\, d^3\vec{r}\,'\, w(\vec{r}, \vec{r}\,')\, \psi^+(\vec{r})\, \underbrace{\psi(\vec{r})\, \psi^+(\vec{r}\,')}_{[\delta(r-r') + \psi^+(r')\psi(r)]}\, \psi(\vec{r}\,') - \frac{1}{2} \int d^3r\, W(\vec{r}, \vec{r})\, \psi^+(\vec{r})\, \psi(\vec{r}).$$

Now we normal order the field operators for the convention:

$$= \frac{1}{2} \int d^3\vec{r}\, d^3\vec{r}\,'\, w(\vec{r}, \vec{r}\,')\, \psi^+(\vec{r})\, \psi^+(\vec{r}\,')\, \psi(\vec{r}\,')\, \psi(\vec{r}) \qquad \text{— (24)}$$

The anti-commutation of field operators cancels the self-interaction term here - this is expected because two fermions cannot be at the same position.

(H.W. : Show the above term where we have used ordered the operators twice so that '–' sign for fermions also drops out).

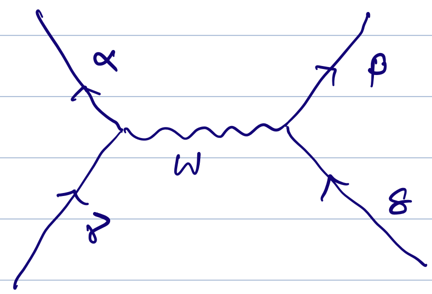
Then we write eq (24) in any basis we want as before:

(Show:) $$= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | w | \gamma\delta \rangle a_\alpha^+ a_\beta^+ a_\delta a_\gamma$$

where $\langle \alpha\beta | w | \gamma\delta \rangle = \int d^3r\, d^3r'\; u_\alpha^*(r)\, u_\beta^*(r')\, w(\vec{r}, \vec{r}')\, u_\gamma(r)\, u_\delta(r')$

This is the main ordering / reordering in the operators, which differ slightly in the matrix element form that we have to keep in mind. Here in the two-body scattering / interaction case, the particle in δ-state goes to β & particle in γ-state goes to α.

- This is represented by the Feynmann diagram as



- This is how we write it. However, when we evaluate it for any physical process for calculation, such as for the electron-electron interaction, we have to consider both possibilities that γ goes to α or β. γ goes to α state at the same position - so this is the direct term, or γ goes to β state exchanging position - this is called the exchange term. But both these terms are included in the formula written in terms of operators, because the commutation/anticommutation between the field operator will take of it.

Density operators:

Apart from the one and two body operators, we will often be using various types of density operators in this course, especially in the momentum space.. We have introduced the local density of particles above in terms of the field operators, for some spin σ, and say orbital α, as

$$\hat{n}_{\alpha,\sigma}(\vec{r}) = \sum_i (\vec{r} - \vec{r}_{i,\alpha,\sigma}) = \hat{\psi}^{+}_{\alpha,\sigma}(r)\ \hat{\psi}_{\alpha\sigma}. \quad \text{--(25)}$$

Let us Fourier transform this density operator to the momentum space as

$$n_{\alpha,\sigma}(\vec{q}) = \int d^3r\ e^{-i\vec{q}.\vec{r}}\ n_{\alpha,\sigma}(\vec{r})$$

$$= \int d^3r\ e^{-i\vec{q}.\vec{r}}\ \hat{\psi}^{+}_{\alpha\sigma}(r)\ \hat{\psi}_{\alpha\sigma}(r)$$

$$= \int d^3r\ e^{-i q.\vec{r}} \overbrace{\frac{1}{\sqrt{V}} \sum_{k} e^{i\vec{k}.\vec{r}}\ a^{+}_{\alpha\sigma}(k)}$$

$$\times \frac{1}{\sqrt{V}} \sum_{k'} e^{i\vec{k}'.\vec{r}}\ a_{\alpha\sigma}(k')$$

$$= \sum_{k,k'} \underbrace{\frac{1}{V}\int d^3r\, e^{i(\vec{k}+\vec{k}'-\vec{q})}}_{\delta(\vec{k}+\vec{k}'-\vec{q})}\ a^{+}_{\alpha\sigma}(k)\ a_{\alpha\sigma}(k')$$

$$= \sum_{k} a^{+}_{\alpha\sigma}(\vec{k}+\vec{q})\ a_{\alpha\sigma}(\vec{k}) \quad \text{--(26)}$$

(here we have redefined some dummy indices).

This is the local density in real space, whose Fourier components in the momentum space gives density waves $n_{\alpha\sigma}(\vec{q})$.

- Notice that the $n(\vec{q})$ itself arises from an summation over all k-states. We can define a local density in momentum space, called the momentum density, as

$$n_{\alpha\sigma}(\vec{k}) = a^{\dagger}_{\alpha\sigma}(\vec{k})\, a_{\alpha\sigma}(\vec{k}) \quad \text{--- (27)}.$$

(Notice that we have used the same symbol $n(q)$ & $n(\vec{k})$ to denote the Fourier component of local-in-$\vec{r}$ density and the momentum density, respectively. Unfortunately, this is what is done in the literature as well and from the context its meaning can be deduced. In this course, we will try to use '$\vec{q}$' to the Fourier transformation of the density and $\vec{k}$ as wave vector of electrons.

The momentum density signifies the occupation density for the Bloch states and it takes the value of (for fermions):

$$n(k) = f(k) \begin{cases} = 0 & \text{for } k > k_F \\ = 1 & \text{for } k \leq k_F \end{cases} \quad \text{at } T=0,$$

ie, its the Fermi-Dirac distribution function at finite temperature.

- $$n(q=0) = \sum_k n(k) = N = \text{total number of electrons in the system } \forall\, \alpha, \sigma. \quad \text{--- (28)}$$

- In first quantization, the local density is

$$n_{\alpha,\sigma}(\vec{r}) = \sum_i \delta(\vec{r}-\vec{r}_{i,\alpha\sigma})$$

$$= \sum_i \sum_q e^{i q\cdot(\vec{r}-\vec{r}_{i,\alpha,\sigma})}$$

$$= \sum_q e^{i q\cdot\vec{r}} \sum_i e^{-i\vec{q}\cdot\vec{r}_{i,\alpha,\sigma}}$$

$$= \sum_q e^{i q\cdot\vec{r}}\, n_{\alpha,\sigma}(\vec{q}) \qquad \text{from eq (26).}$$

Therefore, $$n_{\alpha,q}(\vec{q}) = \sum_i e^{-i\vec{q}\cdot\vec{r}_{i,\alpha,\sigma}}. \qquad — (29)$$

This is the fourier components of the density operator in first quantization, which basically to sum over all plane-wave states corresponding to all sites 'i'.

H.W. (1) Write the one-body and two-body operators in terms of momentum space creation/annihilation operators

(2) Express the electronic Hamiltonian in the 2nd quantized form in terms of field operators as well as in terms of momentum space creation/annihilation operators.

(3) Repeat (2) for the nuclei Hamiltonian.

(4) Write the non-interacting wave function in momentum space for a single band electronic structure with two spins at zero temperature.

(5) Write the wave function for a non-interacting bosonic system at zero temperature.