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Project Title

Study of Second Quantisation and BCS Theory of Superconductivity

Submitted By

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Under the Supervision of

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Declaration

I declare here that the report included in this project entitled **"Study of Second Quantisation and BCS Theory of Superconductivity"** is the summer internship carried out by me in the Department of **Physical Sciences**, Indian Institute if Science Education and Researck Kolkata, India from June 5 to July 31, 2020 under the supervision of **Prof. Amit Ghosal**.

In keeping with general practice of reporting scientific observations, due acknowledgments have been made wherever the work described is based on the findings of other investigators.

Student's e-Signature	Place	Date

Certificate

It is certified that summer research work included in the project report entitled **"Study of Second Quantisation and BCS Theory of Superconductivity"** has been carried out by **Ms. Ashmita Panda** under my supervision and guidance.

Signature of Supervisor
(Prof. Amit Ghosal)
Project Supervisor

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Introduction

The discovery of superconductivity by Heike Kammerlingh Onnes and co-workers in 1911 can be considered as one of the most remarkable discoveries in the history of physics. Mercury was the first substance found to be superconducting, at a temperature near 4K.

In 1957, 46 years after the discovery of superconductivity, Bardeen, Cooper and Schrieffer published their fascinating theory, known as the BCS Theory, explaining the properties of superconductors from the first principles.

To study the BCS Theory, we first need to get thorough with the concepts of Operator Formalism in Quantum Mechanics and Second Quantisation. Then, we need to study the Non-Interacting Electron Gas system and the Cooper Problem to derive the BCS Gap Equation.

In this report, I have tried to present the topics as sequentially as I could to ensure smooth flow of the concepts involved.

I. Operator Formalism in Quantum Mechanics

In Quantum Mechanics, the state of a particle is not defined by using the conventional classical variables of $\vec{r}$ and $\vec{p}$. The mathematical structure of quantum mechanics is based on the concept of 'Operators', especially Linear Operators.

An operator is a function or a mapping which acts on elements of one space to produce elements of another space.
An operator, say L, can be termed as a Linear Operator, if it obeys the following ($|X\rangle$, $|Y\rangle$ are ket vectors, a and b are scalars) :

- $L(a|X\rangle) = a(L|X\rangle)$ (homogeneity of degree 1, i.e., scalar multiplication)
- $L\{a|X\rangle + b|Y\rangle\} = a(L|X\rangle) + b(L|Y\rangle)$ (additivity)

Isolated quantum states are defined using wavefunctions, $|\Psi\rangle$ such that :

- $\iiint_{-\infty}^{+\infty} |\Psi(\boldsymbol{r}, t)|^2 dV < \infty$ (square-integrable)
- $\iiint_{-\infty}^{+\infty} |\Psi(\boldsymbol{r}, t)|^2 dV = 1$ (normalizable)

$|\Psi(\boldsymbol{r}, t)|^2$ gives us the probability density of the particle being at position x.
Multiplying the wavefunction with a constant does not give us a new state, but if a linear operator acts upon it, then we obtain a new ket vector which may or may not describe a new

state.

i. Eigen States and Eigen Values

If a linear operator L, acts upon some $|\Psi\rangle$ to produce some scalar multiple of $|\Psi\rangle$

$$L|\Psi\rangle = \lambda|\Psi\rangle$$

then, $|\Psi\rangle$ is called the 'eigen state' of L and λ is called the 'eigen value' of L. The bra vector equivalent of the same is :

$$\langle\Psi|L^\dagger = \langle\Psi|\lambda^*$$

If L is Hermitian, meaning $L^\dagger = L$, then the eigen values are real, and the eigen states can be chosen such that they are orthogonal to each other. The claims can be proved as follows :

a. Proof that the eigen values of a Hermitian operator are real

Let us consider a Hermitian linear operator L and its eigen ket $|\omega\rangle$.

$$L|\omega\rangle = \omega|\omega\rangle$$

Taking the inner product of $\langle\omega|$ and $L|\omega\rangle$:

$$\langle\omega|L|\omega\rangle = \omega\langle\omega|\omega\rangle \qquad \ldots(1)$$

Taking the adjoint of the above equation, we get :

$$\langle\omega|L^\dagger|\omega\rangle = \omega^*\langle\omega|\omega\rangle \qquad \ldots(2)$$

Subtracting 2 from 1 :

$$\langle\omega|L|\omega\rangle - \langle\omega|L^\dagger|\omega\rangle = (\omega - \omega^*)\langle\omega|\omega\rangle$$

As, L is Hermitian, $L = L^\dagger$:

$$0 = (\omega - \omega^*)\langle\omega|\omega\rangle$$

$$\therefore \omega = \omega^*$$

as $\langle\omega|\omega\rangle = 1$

b. Proof that the eigen kets of a Hermitian operator are orthogonal to each other

This is relatively straight forward if the eigen values of the Hermitian linear operator are non-degenrate, i.e., no value is repeated.

Let L be the Hermitian linear operator. Let $|\omega_i\rangle$ and $|\omega_j\rangle$ be the two eigen kets of L, with

corresponding eigen values, $|\omega_i\rangle$ and $|\omega_j\rangle$ respectively.

$$L|\omega_i\rangle = \omega_i|\omega_i\rangle \qquad \ldots(1)$$
$$L|\omega_j\rangle = \omega_j|\omega_j\rangle \qquad \ldots(2)$$

Taking inner product of $\langle\omega_j|$ with 1 and of $\langle\omega_i|$ with 2 :

$$\langle\omega_j|L|\omega_i\rangle = \omega_i\langle\omega_j|\omega_i\rangle \qquad \ldots(3)$$
$$\langle\omega_i|L|\omega_j\rangle = \omega_j\langle\omega_i|\omega_j\rangle \qquad \ldots(4)$$

Taking adjoint of 4 and subtracting it from 3 :

$$\langle\omega_j|L|\omega_i\rangle - \langle\omega_j|L^\dagger|\omega_i\rangle = (\omega_i - \omega_j^*)\langle\omega_j|\omega_i\rangle$$

As $L = L^\dagger$ and $\omega = \omega^*$ (proved earlier), we get :

$$0 = (\omega_i - \omega_j)\langle\omega_j|\omega_i\rangle$$

We know here that $i \neq j$ and $\omega_i \neq \omega_j$, so $\langle\omega_j|\omega_i\rangle$ must be equal to zero. Thus, $|\omega_i\rangle$ and $|\omega_j\rangle$ areorthnormal to each other if the corresponding eigen values are different.

ii. Commutator

The product of two linear operators (say, L and M), LM may or may not be equal to the product ML. If,

$$LM|\Psi\rangle = ML|\Psi\rangle$$

for all $|\Psi\rangle$, then L and M are said to 'commute'. The commutation properties of these two operators can be studied easily by defining a 'commutator', [L,M] by :

$$[L, M] \equiv LM - ML$$

Operators that commute have zero commutator.

In quantum mechanics, $\vec{r}$ and $\vec{p}$ are replaced by their respective operators.

$\boldsymbol{r} \rightarrow$ position operator $\mathbf{r}$ (multiplicative operator)
$\boldsymbol{p} \rightarrow$ momentum operator : $-i\hbar\nabla$ (differential operator)

Studying the commutation properties of the position and momentum operator, we observe that :

$$[p_x, x] = [p_y, y] \quad = [p_z, z] = -i\hbar$$
$$[p_x, y] = [p_x, z] \quad = [p_y, x] = [p_y, z] \quad = [p_z, x] = [p_z, y] \quad = 0$$

a. $[\boldsymbol{p_x}, \boldsymbol{x}] = \boldsymbol{-i\hbar}$

Operating the commutator $[p_x, x]$ on some wave function $|\Psi\rangle$:

$$\begin{aligned}
[p_x, x]|\Psi\rangle &= [p_x x - x p_x]|\Psi\rangle \\
&= -i\hbar\frac{\partial(x|\Psi\rangle)}{\partial x} + xi\hbar\frac{\partial(|\Psi\rangle)}{\partial x} \\
&= -i\hbar\left\{|\Psi\rangle\frac{\partial x}{\partial x} + x\frac{\partial(|\Psi\rangle)}{\partial x}\right\} + i\hbar x\frac{\partial(|\Psi\rangle)}{\partial x} \\
&= -i\hbar|\Psi\rangle - i\hbar x\frac{\partial(|\Psi\rangle)}{\partial x} + i\hbar x\frac{\partial(|\Psi\rangle)}{\partial x} \\
&= -i\hbar|\Psi\rangle \\
\therefore [\boldsymbol{p_x}, \boldsymbol{x}] &= \boldsymbol{-i\hbar}
\end{aligned}$$

b. $[\boldsymbol{p_x}, \boldsymbol{y}] = \boldsymbol{0}$

Operating the commutator $[p_x, y]$ on some wave function $|\Psi\rangle$:

$$\begin{aligned}
[p_x, y]|\Psi\rangle &= [p_x y - y p_x]|\Psi\rangle \\
&= -i\hbar\frac{\partial(y|\Psi\rangle)}{\partial x} + yi\hbar\frac{\partial(|\Psi\rangle)}{\partial x} \\
&= -i\hbar\left\{|\Psi\rangle\frac{\partial y}{\partial x} + y\frac{\partial(|\Psi\rangle)}{\partial x}\right\} + i\hbar y\frac{\partial(|\Psi\rangle)}{\partial x} \\
&= 0 - i\hbar y\frac{\partial(|\Psi\rangle)}{\partial x} + i\hbar y\frac{\partial(|\Psi\rangle)}{\partial x} \\
&= 0 \\
\therefore [\boldsymbol{p_x}, \boldsymbol{y}] &= \boldsymbol{0}
\end{aligned}$$

iii. Angular Momentum Operator

Angular momentum is one of the fundamental characteristics of motion, even in quantum mechanics. In classical mechanics, we define angular momentum (L) as :

$$\begin{aligned}
\vec{L} &= \vec{r} \times \vec{p} \\
L_x &= y p_z - z p_y \\
L_y &= z p_x - x p_z \\
L_z &= x p_y - y p_x
\end{aligned}$$

In quantum mechanics, angular momentum is analogous to the classical formulation, with p_x, p_y and p_z being replaced by their operator formalism. Thus :

$$L_x = -i\hbar\left[y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right]$$

$$L_y = -i\hbar\left[z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right]$$
$$L_z = -i\hbar\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right]$$

The total angular momentum L can be related to L_x, L_y and L_z by :

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

Studying the commutation properties of these operators we obtain :

$$[L_x, L_y] = i\hbar L_z$$
$$[L_y, L_z] = i\hbar L_x$$
$$[L_z, L_x] = i\hbar L_y$$

We also observe that total angular momentum commutes with all of its individual components,

$$[L^2, L_x] = [L^2, L_y] = [L^2, L_z] = 0$$

a. $[\boldsymbol{L_x, L_y}] = \boldsymbol{i\hbar L_z}$

All the commutator of this form can be derived in a similar manner.

$$[L_x, L_y] = L_xL_y - L_yL_x$$

Calculating L_xL_y and L_yL_x individually :

$$\begin{aligned} L_xL_y &= (i\hbar)^2\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ &= -\hbar^2\left[y\frac{\partial}{\partial z}\left(z\frac{\partial}{\partial x}\right) - y\frac{\partial}{\partial z}\left(x\frac{\partial}{\partial z}\right) - z\frac{\partial}{\partial y}\left(z\frac{\partial}{\partial x}\right) + z\frac{\partial}{\partial y}\left(x\frac{\partial}{\partial z}\right)\right] \\ &= -\hbar^2\left[y\frac{\partial}{\partial x} + yz\frac{\partial^2}{\partial z\partial x} - yx\frac{\partial^2}{\partial z^2} - z^2\frac{\partial^2}{\partial y\partial x} + zx\frac{\partial^2}{\partial y\partial x}\right] \end{aligned}$$

$$\begin{aligned} L_yL_x &= (i\hbar)^2\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ &= -\hbar^2\left[z\frac{\partial}{\partial x}\left(y\frac{\partial}{\partial z}\right) - z\frac{\partial}{\partial x}\left(z\frac{\partial}{\partial y}\right) - x\frac{\partial}{\partial z}\left(y\frac{\partial}{\partial z}\right) + x\frac{\partial}{\partial z}\left(z\frac{\partial}{\partial y}\right)\right] \\ &= -\hbar^2\left[zy\frac{\partial^2}{\partial x\partial z} - z^2\frac{\partial^2}{\partial x\partial y} - xy\frac{\partial^2}{\partial z^2} + x\frac{\partial}{\partial y} + xz\frac{\partial^2}{\partial z\partial y}\right] \end{aligned}$$

$$L_xL_y - L_yL_x = -\hbar^2\left[y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right] = \hbar^2\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right] = (i\hbar)(-i\hbar)\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right]$$

$$\therefore [\boldsymbol{L_x, L_y}] = \boldsymbol{i\hbar L_z}$$

b. $[\boldsymbol{L^2, L_x}] = \boldsymbol{0}$

All the commutator of this form can be derived in a similar manner.

$$[L^2, L_x] = [L_x^2 + L_y^2 + L_z^2, L_x] = [L_x^2, L_x] + [L_y^2, L_x] + [L_z^2, L_x]$$

Using a $[AB, C] = A[B, C] + [A, C]B$ which can be proved easily, we get :

$$\begin{aligned}
[L_x^2, L_x] &= L_x[L_x, L_x] + [L_x, L_x]L_x = L_x.0 + 0.L_x = 0 \\
[L_y^2, L_x] &= L_y[L_y, L_x] + [L_y, L_x]L_y = -i\hbar L_y L_z - i\hbar L_z L_y \\
[L_z^2, L_x] &= L_z[L_z, L_x] + [L_z, L_x]L_z = i\hbar L_z L_y + i\hbar L_y L_z \\
\implies [L^2, L_x] &= 0 - i\hbar L_y L_z - i\hbar L_z L_y + i\hbar L_z L_y + i\hbar L_y L_z \\
\therefore [\boldsymbol{L^2, L_x}] &= \boldsymbol{0}
\end{aligned}$$

c. Eigen values of angular momentum operators

We can obtain eigen values of the angular momentum operators without considering any particular wave function by studying the form and properties of its commutators. To do so, we define two new operators, 'U' and 'D'.

$$\begin{aligned}
U &\equiv L_x + iL_y \\
D &\equiv L_x - iL_y
\end{aligned}$$

We immediately observe that these operators are not Hermitian, so they donot represent any measurable physical quantities.
Multiplying the operators we obtain :

$$\begin{aligned}
UD &= \big(L_x + iL_y\big)\big(L_x - iL_y\big) = L_x^2 + L_y^2 - i[L_x L_y - L_y L_x] \\
&= L_x^2 + L_y^2 - i[L_x, L_y] = L_x^2 + L_y^2 + \hbar L_z = L^2 - L_z^2 + \hbar L_z
\end{aligned}$$

We can similarly obtain DU and write :

$$\begin{aligned}
UD &= L^2 - L_z^2 + \hbar L_z \\
DU &= L^2 - L_z^2 - \hbar L_z
\end{aligned}$$

Considering the commutator of U and D with the operator L_z, we obtain :

$$\begin{aligned}
[L_z, U] &= [L_z, L_x] + i[L_z, L_y] = i\hbar L_y + \hbar L_x = \hbar U \\
[L_z, D] &= [L_z, L_x] - i[L_z, L_y] = i\hbar L_y - \hbar L_x = -\hbar D
\end{aligned}$$

Also, L^2 commutes with both U and D individually as it commutes with each both L_x and L_y.

$$[L^2, U] = [L^2, L_x] + i[L^2, L_y] = 0 = [L^2, L_x] - i[L^2, L_y] = [L^2, D]$$

Thus we can write $L^2U = UL^2$ and $L^2D = DL^2$.

If two operators commute with each other, then they share a set of common eigen kets. Let $|\Psi\rangle$ be an eigen ket of one such set. Considering L^2 and L_z which commute, we can write :

$$L^2|\Psi\rangle = a|\Psi\rangle$$
$$L_z|\Psi\rangle = b|\Psi\rangle$$

where, 'a' and 'b' are integers.
Now, we consider a new eigen ket $|\Psi_1\rangle$ such that, $|\Psi_1\rangle = U|\Psi\rangle$. So,

$$L^2|\Psi_1\rangle = L^2U|\Psi\rangle = UL^2|\Psi\rangle = Ua|\Psi\rangle = aU|\Psi\rangle = a|\Psi_1\rangle$$

Thus, $|\psi_1\rangle$ is also an eigen ket of L^2 with the same eigen value 'a'.
Now considerig L_z :

$$\begin{aligned} L_z|\Psi_1\rangle &= L_zU|\Psi\rangle = (\hbar U + UL_z)|\Psi\rangle \qquad \Big(\because [L_z, U] = \hbar U\Big) \\ &= \hbar U|\Psi\rangle + UL_z|\Psi\rangle \\ &= \hbar|\Psi_1\rangle + Ub|\Psi\rangle \\ &= \hbar|\Psi_1\rangle + b|\Psi_1\rangle \\ \therefore L_z|\Psi_1\rangle &= (\hbar + b)|\Psi_1\rangle \end{aligned}$$

Thus, $|\Psi_1\rangle$ is also an eigen ket of L_z but with an eigen value of $\hbar + b$. The eigen value get increased by $\hbar$ in moving from $|\Psi\rangle$ to $|\Psi_1\rangle$ by the action of U. D acts in the exactly opposite way, i.e., by decreasing the eigen value by $\hbar$ in moving from $|\Psi\rangle$ to $|\Psi_1\rangle$. IN both cases, the eigen value of L^2 operator remains unchanged.
Thus, U and D are known as 'Ladder Operators'.

We could apply them repeatedly to any common eigen ket to generate a series of eigen kets with eigen values changing by a factor of $\pm\hbar$ for L_z and remaining unchanged for L^2. But we also need to take into consideration the physical constraints upon the operators. As $L^2 = L_x^2 + L_y^2 + L_z^2$, b^2 cannot exceed a for real values of z-component. So, $b^2 \leq a$.

Let b have a maximum value, c. So, $c^2 \leq a$. But it is clear that $(c + \hbar)^2 > a$. Then the eigen ket corresponding to $c + \hbar$ must be an unphysical state. So we set it equal to the zero ket, $|\phi\rangle$.

Let $|\Psi_u\rangle$ be the eigen ket corresponding to c^{th} eigen value.

$$L_z U|\Psi_u\rangle = (c+\hbar)U|\Psi_u\rangle$$

But $U|\Psi_u\rangle = |\phi\rangle$. If we use $DU|\Psi_u\rangle = (L^2 - L_z^2 - \hbar L_z)|\Psi_u\rangle$, we obtain :

$$\begin{aligned}
DU|\Psi_u\rangle &= (a - c^2 - \hbar c)|\Psi_u\rangle \\
D|\phi\rangle &= (a - c^2 - \hbar c)|\Psi_u\rangle \\
|\phi\rangle &= (a - c^2 - \hbar c)|\Psi_u\rangle \\
0 &= (a - c^2 - \hbar c) \qquad \Big(\because |\Psi_u\rangle \neq |\phi\rangle\Big) \\
\therefore &\boxed{a = c(c+\hbar)}
\end{aligned}$$

Repeating the operation n times with D operator this time, let us assume we reach the lowest possible $|\Psi_d\rangle$ which corresponds to a physical state. Any eigen ket with obtained by operating D on $|\Psi_d\rangle$ must be an unphysical state, thus equal to the zero ket, $|\phi\rangle$.

$$L_z D|\Psi_d\rangle = (c - n\hbar)D|\Psi_d\rangle$$

But $D|\Psi_d\rangle = |\phi\rangle$. If we use $UD|\Psi_d\rangle = (L^2 - L_z^2 + \hbar L_z)|\Psi_d\rangle$, we obtain :

$$\begin{aligned}
UD|\Psi_d\rangle &= \Big\{a - (c-n\hbar)^2 + \hbar(c-n\hbar)\Big\}|\Psi_d\rangle \\
U|\phi\rangle &= \Big\{a - (c-n\hbar)^2 + \hbar(c-n\hbar)\Big\}|\Psi_d\rangle \\
|\phi\rangle &= \Big\{a - (c-n\hbar)^2 + \hbar(c-n\hbar)\Big\}|\Psi_d\rangle \\
0 &= \Big\{a - (c-n\hbar)^2 + \hbar(c-n\hbar)\Big\} \qquad \Big(\because |\Psi_u\rangle \neq |\phi\rangle\Big) \\
\therefore a &= (c-n\hbar)^2 - \hbar(c-n\hbar)
\end{aligned}$$

Equating both values of a, we get :

$$\begin{aligned}
(c-\hbar)^2 - \hbar(c-n\hbar) &= c^2 + c\hbar \\
\implies \cancel{c^2} - 2nc\hbar + n^2\hbar^2 - \hbar c + n\hbar^2 &= \cancel{c^2} + c\hbar \\
\implies n^2\hbar^2 + n\hbar^2 - 2nc\hbar - 2\hbar &= 0 \\
\implies \hbar^2 n\cancel{(n+1)} &= 2\hbar c\cancel{(n+1)} \\
\therefore &\boxed{c = \frac{n\hbar}{2}}
\end{aligned}$$

c forms the eigen values of L_z operator. For a given n, let us define $\frac{n}{2} \equiv l$
So, the eigen values of L_z operator are given by :

$$l\hbar,\ (l-1)\hbar,\ (l-2)\hbar,\ \ldots\ldots\ldots,\ -l\hbar$$

For all these states, $a = c(c + \hbar)$, where $c = l\hbar$. So,

$$a = (l\hbar)^2 + l\hbar^2 = l^2\hbar^2 + l\hbar^2$$
$$\therefore \boxed{a = l(l+1)\hbar^2}$$

iv. Annihilation and Creation Operator

Let us consider the Hamiltonian of a one-dimensional simple harmonic oscillator of mass 'm'. The potential associated with it is $V = \frac{1}{2}m\omega^2x^2$.

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

We know from previous sections that the corresponding operators, p and x donot commute and $[p, x] = -i\hbar$. Let us two operator analogous to ladder operators,

$$A \equiv \sqrt{\frac{m\omega}{2}}x + \frac{ip}{\sqrt{2m\omega}}$$
$$A^\dagger \equiv \sqrt{\frac{m\omega}{2}}x - \frac{ip}{\sqrt{2m\omega}}$$

We immediately observe that A and $A^\dagger$ are not Hermitian operators and so they donot represent any measurable physical operators. Now, considering $AA^\dagger$ and $A^\dagger A$:

$$\begin{aligned} AA^\dagger &= \left[\sqrt{\frac{m\omega}{2}}x + \frac{ip}{\sqrt{2m\omega}}\right]\left[\sqrt{\frac{m\omega}{2}}x - \frac{ip}{\sqrt{2m\omega}}\right] \\ &= \frac{m\omega}{2}x^2 - \frac{ixp}{2} + \frac{ixp}{2} + \frac{p^2}{2m\omega} \\ &= \frac{H}{\omega} + \frac{i}{2}[px - xp] \end{aligned}$$
$$\boxed{\therefore AA^\dagger = \frac{H}{\omega} + \frac{i}{2}[p, x]}$$
$$\begin{aligned} A^\dagger A &= \left[\sqrt{\frac{m\omega}{2}}x - \frac{ip}{\sqrt{2m\omega}}\right]\left[\sqrt{\frac{m\omega}{2}}x + \frac{ip}{\sqrt{2m\omega}}\right] \\ &= \frac{m\omega}{2}x^2 + \frac{ixp}{2} - \frac{ixp}{2} + \frac{p^2}{2m\omega} \\ &= \frac{H}{\omega} - \frac{i}{2}[px - xp] \end{aligned}$$
$$\boxed{\therefore A^\dagger A = \frac{H}{\omega} - \frac{i}{2}[p, x]}$$

We immediately observe that :

$$\boxed{\therefore H = \frac{\omega}{2}(A^\dagger A + AA^\dagger)}$$

We also observe that $[A, A^\dagger] = \hbar$.
Now, taking commutators of H with A and $A^\dagger$, we get :

$$[H, A] = -\hbar\omega A$$
$$[H, A^\dagger] = \hbar\omega A^\dagger$$

a. $[H, A] = -\hbar\omega A$

$[H, A^\dagger] = \hbar\omega A^\dagger$ can also be obtained using similar process.

$$\begin{aligned}[H, A] &= \left[\frac{\omega}{2}(A^\dagger A + AA^\dagger), A\right] \\ &= \frac{\omega}{2}\Big\{[A^\dagger A, A] + [AA^\dagger, A]\Big\}\end{aligned}$$

Using the property of commutators $[XY, Z] = X[Y, Z] + [X, Z]Y$ and $[X, X] = 0$ we get :

$$\begin{aligned}[H, A] &= \frac{\omega}{2}\Big\{A^\dagger \cancelto{0}{[A, A]} + [A^\dagger, A]A + A[A^\dagger, A] + \cancelto{0}{[A, A]}A^\dagger\Big\} \\ &= \frac{\omega}{2}\Big\{[A^\dagger, A]A + A[A^\dagger, A]\Big\} \\ &= \frac{\omega}{2}\Big\{ - [A, A^\dagger] - A[A, A^\dagger]\Big\} \\ &= \frac{\omega}{2}\{-\hbar A - \hbar A\} = \frac{-2\omega\hbar A}{2}\end{aligned}$$
$$\boxed{\therefore [H, A] = -\hbar\omega A}$$

b. Energy Spectrum of Simple Harmonic Oscillator

Before we start discussing the energy spectrum of SHO, we need to prove a result which we will use later.

Statement :- $\langle\psi|B^2|\psi\rangle \geq 0$ if B is a Hermitian Operator.
Proof :- We can start by re-writing $\langle\psi|B^2|\psi\rangle$: -

$$\langle\psi|B^2|\psi\rangle = \langle\psi|B \times 1 \times B|\psi\rangle$$

Replacing 1 with the identity operator, we obtain :

$$\begin{aligned}\langle\psi|B^2|\psi\rangle &= \sum_i \langle\psi|B|\phi_i\rangle\langle\phi_i|B|\psi\rangle \\ &= \sum_i \langle\psi|B|\phi_i\rangle\Big(\langle\phi_i|B|\psi\rangle^*\Big)^* \\ &= \sum_i \langle\psi|B|\phi_i\rangle\Big(\langle\psi|B^\dagger|\phi_i\rangle\Big)^*\end{aligned}$$

$$= \sum_i \langle\psi|B|\phi_i\rangle\langle\psi|B|\phi_i\rangle^* \qquad [\because B = B^\dagger]$$

As in Hilbert space, the norm of all quantities is positive definite, we can say :

$$\boxed{\therefore \langle\psi|B^2|\psi\rangle = \sum_i |\langle\psi|B|\phi_i\rangle|^2 \geq 0}$$

Writing the original expression for H, and recalling the discussion on x and p operators done previously,

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

we immediately see that H is the sum of two operator of the form B^2 discussed above, as x and p operators are both hermitian. So, we can say $\langle\psi|H|\psi\rangle \geq 0$.

Let $|E_n\rangle$ denote the n^{th} energy state of the Simple Harmonic Oscillator. So,

$$H|E_n\rangle = E_n|E_n\rangle$$

Let us consider the state $A|E_n\rangle$.

$$\begin{aligned} HA|E_n\rangle &= AH|E_n\rangle - \hbar\omega A|E_n\rangle \qquad [\because [H, A] = -\hbar\omega A] \\ &= AE_n|E_n\rangle - \hbar\omega A|E_n\rangle \\ &= (E_n - \hbar\omega)A|E_n\rangle \end{aligned}$$

Thus, we observe that $A|E_n\rangle$ is still an eigen state of H, but with eigen value reduced by $\hbar\omega$. A posseses the property of reducing the energy of the state by $\hbar\omega$, i.e., by one quantum of excitation energy for the oscillator. So, A is called the Annihilation Operator.

Repeated application of A, say m times, produces a state which has energy $m\hbar\omega$ less than the original state.

$$A^m|E_n\rangle = c_n c_{n-1} \ldots c_{n-m+1}|E_n - m\hbar\omega\rangle$$

$A^\dagger$ creates an additional quantum of energy $\hbar\omega$ for the oscillator each time is acts upon $|\xi_n\rangle$, so it is called the Creation Operator.

Repeated application of $A^\dagger$, say m times, produces a state which has energy $m\hbar\omega$ more than the original state.

$$(A^\dagger)^m|E_n\rangle = d_n d_{n+1} \ldots d_{n+m-1}|E_n + m\hbar\omega\rangle$$

Using the result already proved earlier($\langle\psi|H|\psi\rangle \geq 0$), we know that there must be some lowest or ground state.
Let E_0 be the lowest eigen value and $|0\rangle$ be the corresponding eigen ket. We set $\boldsymbol{A|0\rangle = |\phi\rangle}$

as any further lowering must lead to an unphysical state.

$$\begin{aligned} H|0\rangle &= \frac{1}{2}\omega(A^\dagger A + AA^\dagger)|0\rangle \\ &= \frac{\omega}{2}\big(A^\dagger A|0\rangle + AA^\dagger|0\rangle\big) \\ &= \frac{\omega}{2}\big(A^\dagger A|0\rangle + A^\dagger A|0\rangle + \hbar|0\rangle\big) \qquad (\because [A, A^\dagger] = \hbar) \\ &= \frac{\omega}{2}\big(A^\dagger|\phi\rangle + A^\dagger|\phi\rangle + \hbar|0\rangle \\ \boxed{\therefore H|0\rangle = \frac{\hbar\omega}{2}|0\rangle} \end{aligned}$$

Thus, the lowest ground state of energy is $\frac{\hbar\omega}{2}$.

Thus, the allowed energy values and their corresponding eigen states are :

$$\frac{\hbar\omega}{2} \to |0\rangle, \frac{3\hbar\omega}{2} \to A^\dagger|0\rangle, \frac{5\hbar\omega}{2} \to (A^\dagger)^2|0\rangle, \ldots, (m+\frac{1}{2})\hbar\omega \to (A^\dagger)^m|0\rangle$$

c. Normalization of the eigen states

We will use the relations $[A, A^\dagger]$ and $A|0\rangle = |\phi\rangle$ to determine the normalization constants of A and $A^\dagger$, $c_n, c_{n-1}, \ldots, c_{n-m+1}$ and $d_n, d_{n+1}, \ldots, d_{n+m-1}$ respectively.

Let us consider $A^m(A^\dagger)^m$:

$$\begin{aligned} A^m(A^\dagger)^m &= A^{m-1}AA^\dagger(A^\dagger)^{m-1} \\ &= A^{m-1}(AA^\dagger)(A^\dagger)^{m-1} \\ &= A^{m-1}(A^\dagger A + \hbar)(A^\dagger)^{m-1} \\ &= A^{m-1}A^\dagger A(A^\dagger)^{m-1} + A^{m-1}\hbar(A^\dagger)^{m-1} \\ &= A^{m-1}(A^\dagger)(AA^\dagger)(A^\dagger)^{m-2} + \hbar A^{m-1}(A^\dagger)^{m-1} \\ &= A^{m-1}(A^\dagger)(AA^\dagger + \hbar)(A^\dagger)^{m-2} + \hbar A^{m-1}(A^\dagger)^{m-1} \\ &= A^{m-1}(A^\dagger)^2A(A^\dagger)^{m-2} + 2\hbar A^{m-1}(A^\dagger)^{m-1} \\ &\vdots \quad \textit{repeating m-2 times} \\ \therefore A^m(A^\dagger)^m &= A^{m-1}(A^\dagger)^m A + m\hbar A^{m-1}(A^\dagger)^{m-1} \end{aligned}$$

Taking the expectation values for ground state :

$$\begin{aligned} \langle 0|A^m(A^\dagger)^m|0\rangle &= \rangle 0|A^{m-1}(A^\dagger)^m A + m\hbar A^{m-1}(A^\dagger)^{m-1}|0\rangle \\ &= \langle 0|A^m(A^\dagger)^m A|0\rangle + m\hbar\langle 0|A^{m-1}(A^\dagger)^{m-1}|0\rangle \\ &= \langle 0|\phi\rangle + m\hbar\langle 0|A^{m-1}(A^\dagger)^{m-1}|0\rangle \\ \therefore 0|A^m(A^\dagger)^m|0\rangle &= 0|A^{m-1}(A^\dagger)^{m-1}|0\rangle \end{aligned}$$

$$\implies |(A^\dagger)^m|0\rangle|^2 = m\hbar|(A^\dagger)^{m-1}|0\rangle|^2$$
$$\implies |d_0|^2|d_1|^2\ldots|d_{m-1}|^2 = m\hbar|d_0|^2|d_1|^2\ldots|d_{m-2}|^2$$
$$\implies |d_{m-1}|^2 = m\hbar$$
$$\boxed{\therefore d_m = \sqrt{(m+1)\hbar}}$$

Now, taking the commutator :

$$[A, A^\dagger]|n\rangle = AA^\dagger|n\rangle - A^\dagger A|n\rangle$$
$$\implies \hbar|n\rangle = A\sqrt{(n+1)\hbar}|(n+1)\rangle - A^\dagger c_n|(n-1)\rangle$$
$$\implies \hbar|n\rangle = \sqrt{(n+1)\hbar}A|(n+1)\rangle - c_n A^\dagger|(n-1)\rangle$$
$$\implies \hbar|n\rangle = \sqrt{(n+1)\hbar}c_{n+1}|n\rangle - c_n\sqrt{n\hbar}|n\rangle$$
$$\implies \hbar = c_{n+1}\sqrt{(n+1)\hbar} - c_n\sqrt{n\hbar}$$
$$\boxed{\therefore c_n = \sqrt{n\hbar}}$$

II. First Quantisation of Many-Body Systems

The physical world consists of many particles interacting together to form a system.
First quantisation deals with the quantisation of the motion of the particles. To get an accurate description of such systems, we need to include the inter-particle potential and solve the Schrodinger's equation for many-body system.
But to obtain a direct solution of many particle Schrodinger's equation is nearly impossible. So, we resort to indirect methods.

On the other hand, second quantisation elevates the quantum field to the status of operators. It is essential to describe the creation and destruction of particles in a relativistic theory.
The Hamiltonian for many particle system can be written as :

$$H = \sum_{k=1}^{N} T(x_k) + \frac{1}{2}\sum_{k\neq l=1}^{N} V(x_k, x_l)$$

where, T is the kinetic energy, V is the potential energy and x_k denotes the k^{th} particle coordinates (includes spatial coordinate x_k and any discrete variables like z component of spin for ferminons, etc).
So, the time dependent Schrodinger's equation for many particles is given as :

$$i\hbar\frac{\partial}{\partial t}\Psi(x_1, x_2, \ldots, x_N, t) = H\Psi(x_1, x_2, \ldots, x_N, t)$$

Here, we will use $\psi_{\xi_k}(x_k)$ to denote the single particle wave functions. ξ_k represents a complete set of single particle quantum numbers. This set could be infinite. We conveniently assume that this set of eigen values, possibly infinite, is ordered and ξ_k runs over it.

i. Basis states for an N-particle system

Let us consider a complete and orthonormal single particle basis : $\left\{\psi_\xi(\vec{r})\right\}$

$$\sum_\xi \psi_\xi^*(\vec{r'})\psi_\xi(\vec{r}) = \delta(\vec{r}-\vec{r'}) \qquad \text{(completeness)}$$

$$\int d\vec{r}\psi_\xi^*(\vec{r})\psi_{\xi'}(\vec{r}) = \delta_{\xi\xi'} \qquad \text{(orthonormality)}$$

Starting with N-particle state $\Psi(r_1, r_2, \ldots, r_N)$ we form $(N-1)$ particle function $A_{\xi_1}(r_2, r_3, \ldots, r_N)$ such that :

$$A_{\xi_1}(r_2, r_3, \ldots, r_N) = \underbrace{\int dr_1 \psi_{\xi_1}^*(r_1)\Psi(r_1, r_2, \ldots, r_N)}_{\text{projecting onto 1 particle basis}}$$

Multiplying $\psi_{\xi_1}(r_1^{'})$ to above equation and summing over n_1 :

$$\begin{aligned}
\sum_{\xi_1} \psi_{\xi_1}(r_1^{'})A_{\xi_1}(r_2, r_3, \ldots, r_N) &= \sum_{\xi_1} \psi_{\xi_1}(r_1^{'}) \int dr_1 \psi_{\xi_1}^* \Psi(r_1, r_2, \ldots, r_N) \\
&= \int dr_1 \Psi(r_1, r_2, \ldots, r_N) \sum_{\xi_1} \psi_{\xi_1}(r_1^{'})\psi_{\xi_1}^*(r_1) \\
&= \int dr_1 \Psi(r_1, r_2, \ldots, r_N)\delta(r_1 - r_1^{'}) \qquad [\because \text{Completeness Condition}]
\end{aligned}$$

$$\boxed{\therefore \Psi(r_1^{'}, r_2, \ldots, r_N) = \sum_{\xi_1} \psi_{\xi_1}(r_1^{'})A_{\xi_1}(r_2, r_3, \ldots, r_N)}$$

Now we define $A_{\xi_1\xi_2}(r_3, r_4, \ldots, r_N)$ from $A_{\xi_1}(r_2, r_3, \ldots, r_N)$ and projecting onto the 1 particle basis $\psi_{\xi_2}(r_2)$:

$$A_{\xi_1\xi_2}(r_3, r_4, \ldots, r_N) = \int dr_2 \psi_{\xi_2}^*(r_2)A_{\xi_1}(r_2, r_3, \ldots, r_N)$$

Multiplying throughout by $\psi_{\xi_2}(r_2^{'})$ and summing over n_2 :

$$\begin{aligned}
\sum_{\xi_2} \psi_{\xi_2}(r_2^{'})A_{\xi_1\xi_2}(r_3, r_4, \ldots, r_N) &= \sum_{\xi_2} \psi_{\xi_2}(r_2^{'}) \int dr_2 \psi_{\xi_2}^*(r_2)A_{\xi_1}(r_2, r_3, \ldots, r_N) \\
&= \int dr_2 A_{\xi_1}(r_2, r_3, \ldots, r_N) \sum_{\xi_2} \psi_{\xi_2}(r_2^{'})\psi_{\xi_2}^*(r_2) \\
&= \int dr_2 A_{\xi_1}(r_2, r_3, \ldots, r_N)\delta(r_2 - r_2^{'}) \qquad [\because \text{Completeness Condition}] \\
&= A_{\xi_1}(r_2^{'}, r_3, \ldots, r_N)
\end{aligned}$$

$$\boxed{\therefore \sum_{\xi_2} \psi_{\xi_2}(r_2^{'})A_{\xi_1\xi_2}(r_3, r_4, \ldots, r_N) = \int dr_1 \psi_{\xi_1}^*(r_1)\Psi(r_1, r_2^{'}, \ldots, r_N)}$$

Multiplying throughout by $\psi^*_{\xi_1}(r_1^{'})$ and summing over n_1 :

$$\sum_{\xi_1}\sum_{\xi_2}\psi_{\xi_1}(r_1^{'})\psi_{\xi_2}(r_2^{'})A_{\xi_1\xi_2}(r_3,r_4,\ldots,r_N) = \sum_{\xi_1}\psi_{\xi_1}(r_1^{'})\int dr_1\psi^*_{\xi_1}(r_1)\Psi(r_1,r_2^{'},r_3,\ldots,r_N)$$

$$= \int dr_1\Psi(r_1,r_2^{'},r_3,\ldots,r_N)\sum_{\xi_1}\psi_{\xi_1}(r_1^{'})\psi^*_{\xi_1}(r_1)$$

$$= \int dr_1\Psi(r_1,r_2^{'},r_3,\ldots,r_N)\delta(r_1-r_1^{'}) \qquad [\because \text{Completeness }]$$

$$\boxed{\therefore \Psi(r_1^{'},r_2^{'},r_3,r_4,\ldots,r_N) = \sum_{\xi_1,\xi_2}\psi_{\xi_1}(r_1^{'})\psi_{\xi_2}(r_2^{'})A_{\xi_1\xi_2}(r_3,r_4,\ldots,r_N)}$$

Similarly, repeating this process another $n-2$ times, we obtain :

$$\Psi(r_1^{'},r_2^{'},\ldots,r_N^{'}) = \sum_{\xi_1,\xi_2,\ldots,\xi_N} A_{\xi_1\xi_2\ldots\xi_N}\psi_{\xi_1}(r_1^{'})\psi_{\xi_2}(r_2^{'})\ldots\psi_{\xi_N}(r_N^{'})$$

$A_{\xi_1\xi_2\ldots\xi_N}$ is a complex number independent of all $r_i^{'}$s. We can replace all $r_i^{'}$ with r_i as now they are essentially dummy variables. So,

$$\boxed{\Psi(r_1,r_2,r_3,r_4,\ldots,r_N) = \sum_{\xi_1,\xi_2,\ldots,\xi_N} A_{\xi_1\xi_2\ldots\xi_N}\psi_{\xi_1}(r_1)\psi_{\xi_2}(r_2)\ldots\psi_{\xi_N}(r_N)} \tag{1}$$

We can also write $A_{\xi_1\xi_2\ldots\xi_N}$ as $A(\xi_1,\xi_2,\ldots,\xi_N)$. If we want to denote the time dependence of the many particle wave function, we observe it must appear in the coefficients, making :

$$A(\xi_1,\xi_2,\ldots,\xi_N) \longrightarrow A(\xi_1,\xi_2,\ldots,\xi_N,t)$$

as all $\psi_{\xi_k}(r_k)$ are independent of time.
Thus, basis states for N-particle system can be built from any complete and orthonormal single particle basis states.

ii. Assumptions in Many-Body QM

When formulating N-particle Quantum Mechanics, containing for example, N identical electrons or protons etc, we need to make 3 assumptions apart from the usual postulates of one particle Quantum Mechanics.

a. Assumption1

The single particle wave function is expanded to many particle wave function,

$$\psi(r) \longrightarrow \Psi(r_1,r_2,\ldots,r_N)$$

such that $|\Psi(r_1, r_2, \ldots, r_N)|^2$ gives us the probability of finding N particles in dN-dimensional volume $\left\{ = \prod_{j=1}^{N} d^d r_j \right\}$ surrounding the point $(r_1, r_2, \ldots, r_N)$ in a dN-dimensional configuration space.

b. Assumption 2

Identical particles, i.e., particles characterized by the same quantum numbers and physical properties like mass, charge etc are in principle, indistinguishable.

Indistinguishability : If two coordinates of a N particle wave function are interchanged, the same physical state or wave function results, i.e. the two wave functions differing only by a swap of a pair of coordinates can differ atmost by a factor λ, which is a scalar. So,

$$\Psi(r_1, r_2, \ldots, r_j, \ldots, r_k, \ldots, r_N) = \lambda \Psi(r_1, r_2, \ldots, r_k, \ldots, r_j, \ldots, r_N)$$

Another interchange of the same pair gives us :

$$\Psi(r_1, r_2, \ldots, r_j, \ldots, r_k, \ldots, r_N) = \lambda \Psi(r_1, r_2, \ldots, r_j, \ldots, r_k, \ldots, r_N)$$

So, we get $\lambda^2 = 1$, as two successive identical interactions takes it back to original.
Therefore, $\boxed{\lambda = \pm 1}$ and we can write :

$$\boxed{\Psi(r_1, r_2, \ldots, r_j, \ldots, r_k, \ldots, r_N) = \pm \Psi(r_1, r_2, \ldots, r_k, \ldots, r_j, \ldots, r_N)} \tag{2}$$

Putting this is in (1) :

$$\begin{aligned}
&\Psi(r_1, \ldots, r_j, \ldots, r_k, \ldots, r_N) \\
&\quad = \sum_{\xi_1, \ldots, \xi_j, \ldots, \xi_k, \ldots, \xi_N} A(\xi_1, \ldots, \xi_j, \ldots, \xi_k, \ldots, \xi_N) \psi_{\xi_1}(r_1) \ldots \psi_{\xi_j}(r_j) \ldots \psi_{\xi_k}(r_k) \ldots \psi_{\xi_N}(r_N)
\end{aligned}$$

Putting this is (2) :

$$\begin{aligned}
&\sum_{\xi_1, \ldots, \xi_j, \ldots, \xi_k, \ldots, \xi_N} A(\xi_1, \ldots, \xi_j, \ldots, \xi_k, \ldots, \xi_N) \psi_{\xi_1}(r_1) \ldots \psi_{\xi_j}(r_j) \ldots \psi_{\xi_k}(r_k) \ldots \psi_{\xi_N}(r_N) \\
&\quad = \pm \sum_{\xi_1, \ldots, \xi_k, \ldots, \xi_j, \ldots, \xi_N} A(\xi_1, \ldots, \xi_k, \ldots, \xi_j, \ldots, \xi_N) \psi_{\xi_1}(r_1) \ldots \psi_{\xi_k}(r_k) \ldots \psi_{\xi_j}(r_j) \ldots \psi_{\xi_N}(r_N)
\end{aligned}$$

Multiplying with $\prod_{l=1}^{N} \int \psi^*_{m_l}(r_l) dr_l$ on both sides and using the completeness criteria, we get :

$$\text{LHS} = \sum_{\xi_1, \ldots, \xi_j, \ldots, \xi_k, \ldots, \xi_N} A(\xi_1, \ldots, \xi_j, \ldots, \xi_k, \ldots, \xi_N) \prod_{l=1}^{N} \delta_{m_l n_l} = A(\xi_1, \ldots, \xi_j, \ldots, \xi_k, \xi_N)$$

$$\text{RHS} = \pm \sum_{\xi_1,\ldots,\xi_k,\ldots,\xi_j,\ldots,\xi_N} A(\xi_1,\ldots,\xi_k,\ldots,\xi_j,\ldots,\xi_N) \prod_{l=1}^{N} \delta_{m_l n_l} = \pm A(\xi_1,\ldots,\xi_k,\ldots,\xi_j,\xi_N)$$

So, a necessary and sufficient condition for (2) to be valid is :

$$\boxed{A(\xi_1,\ldots,\xi_j,\ldots,\xi_k,\xi_N) = \pm A(\xi_1,\ldots,\xi_k,\ldots,\xi_j,\xi_N)} \tag{3}$$

Bosons are particles whose many-body wave functions are symmetric under the interchange of any two particles, or equivalently, the expansion of coordinates is symmetric under the interchange of the corresponding quantum numbers. $\boxed{\lambda = 1}$

$$\Psi(r_1, r_2, \ldots, r_j, \ldots, r_k, \ldots, r_N) = \Psi(r_1, r_2, \ldots, r_k, \ldots, r_j, \ldots, r_N)$$
$$A(\xi_1, \xi_2, \ldots, \xi_j, \ldots, \xi_k, \ldots, \xi_N) = A(\xi_1, \xi_2, \ldots, \xi_k, \ldots, \xi_j, \ldots, \xi_N)$$

Ferminons are particles whose many-body wave functions are anti-symmetric under the interchange of the coordinates of any two particles, or equivalently, the expansion of coordinates is anti-symmetricunder the interchange of the corresponding quantum numbers. $\boxed{\lambda = -1}$

$$\Psi(r_1, r_2, \ldots, r_j, \ldots, r_k, \ldots, r_N) = -\Psi(r_1, r_2, \ldots, r_k, \ldots, r_j, \ldots, r_N)$$
$$A(\xi_1, \xi_2, \ldots, \xi_j, \ldots, \xi_k, \ldots, \xi_N) = -A(\xi_1, \xi_2, \ldots, \xi_k, \ldots, \xi_j, \ldots, \xi_N)$$

We can immediately observe that if $r_j = r_k$ then
$\Psi(r_1, r_2, \ldots, r_j, \ldots, r_j, \ldots, r_N) = -\Psi(r_1, r_2, \ldots, r_j, \ldots, r_j, \ldots, r_N)$, implying $\Psi = 0$. Thus, two fermions cannot be in the same position in space (Pauli's Exclusion Principle).
Also, if the particles are identical, then the probability density $|\Psi(r_1, \ldots, r_N)|^2$ must be invariant under arbitrary exchange of coordinates of two particles. Let
$\hat{P}_{jk}\Psi(r_1, r_2, \ldots, r_j, \ldots, r_k, \ldots, r_N) = \Psi(r_1, r_2, \ldots, r_k, \ldots, r_j, \ldots, r_N)$
It must be equal to $\boldsymbol{e^{i\phi}\Psi(r_1, r_2, \ldots, r_j, \ldots, r_k, \ldots, r_N)}$. This way, probability density remains invariant.

$$\text{If } \phi = 0 \implies e^{i\phi} = 1 \implies \text{Boson}$$
$$\text{If } \phi = \pi \implies e^{i\phi} = -1 \implies \text{Fermion}$$
$$\text{If } \phi \neq 0, \pi \implies e^{i\phi} \neq 1, -1 \implies \text{Anyon}$$

c. Assumption 3

The third assumption states that the one and two particle operators defined for one and two-or-more particle states remain unchanged when acting on N-particles.

Let us consider the kinetic energy operator $\boldsymbol{T(r_j, \nabla r_j)}$. We define $T_{\xi_a\xi_b}$ and T_j such that :

$$T_{\xi_a\xi_b} = \int dr_j^{'} \psi_{\xi_b}^*(r_j^{'}) T(r_j^{'}, \nabla r_j^{'}) \psi_{\xi_a}(r_j^{'})$$
$$T_j = \sum_{\xi_a,\xi_b} T_{\xi_a\xi_b} |\psi_{\xi_b}(r_j)\rangle\langle\psi_{\xi_a}(r_j)|$$

Evaluating T_j we obtain :

$$\begin{aligned} T_j &= \sum_{\xi_a,\xi_b} \int dr_j^{'} \psi_{\xi_b}^*(r_j^{'}) T(r_j^{'}, \nabla r_j^{'}) \psi_{\xi_a}(r_j^{'}) \psi_{\xi_b}(r_j) \psi_{\xi_a}^*(r_j) \\ &= \int dr_j^{'} T(r_j^{'}, \nabla r_j^{'}) \sum_{\xi_b} \psi_{\xi_b}^*(r_j^{'}) \psi_{\xi_b}(r_j) \sum_{\xi_a} \psi_{\xi_a}(r_j^{'}) \psi_{\xi_a}^*(r_j) \\ &= \int dr_j^{'} T(r_j^{'}, \nabla r_j^{'}) \delta(r_j^{'} - r_j) \delta(r_j^{'} - r_j) \\ \boxed{\therefore T_j &= T(r_j, \nabla r_j)} \end{aligned}$$

Let the total symmetric kinetic energy operator associated with all the coordinates be :

$$T_{tot} = \sum_{j=1}^{N} T_j$$

If it acts on a many-body wave function $\Psi(r_1, r_2, \ldots, r_N)$ then :

$$\begin{aligned} T_{tot}|\Psi(r_1, r_2, \ldots, r_N)\rangle &= T_{tot} \prod_{k=1}^{N} \sum_{\xi_k} |\psi_{\xi_k}(r_k)\rangle \qquad \text{[Coefficients assumed to be 1]} \\ &= \sum_{j=1}^{N} T_j \prod_{k=1}^{N} \sum_{\xi_k} |\psi_{\xi_k}(r_k)\rangle \\ &= \sum_{j=1}^{N} \sum_{\xi_a,\xi_b} T_{\xi_a\xi_b} |\psi_{\xi_b}(r_j)\rangle\langle\psi_{\xi_a}(r_j)| \prod_{k=1}^{N} \sum_{\xi_k} |\psi_{\xi_k}(r_k)\rangle \\ &= \sum_{j=1}^{N} \sum_{\xi_a,\xi_b} T_{\xi_a\xi_b} |\psi_{\xi_b}(r_j)\rangle\langle\psi_{\xi_a}(r_j)| \sum_{\xi_j} |\psi_{\xi_j}(r_j)\rangle \prod_{k=1\neq j}^{N} \sum_{\xi_k} |\psi_{\xi_k}(r_k) \\ &= \sum_{j=1}^{N} \sum_{\xi_a,\xi_b} T_{\xi_a\xi_b} |\psi_{\xi_b}(r_j)\rangle \sum_{n} \langle\psi_{\xi_a}(r_j)|\psi_{\xi_{n_j}}(r_j)\rangle \prod_{k=1\neq j}^{N} \sum_{\xi_k} |\psi_{\xi_k}(r_k)\rangle \\ &= \sum_{j=1}^{N} \sum_{\xi_a,\xi_b} T_{\xi_a\xi_b} |\psi_{\xi_b}(r_j)\rangle \delta_{\xi_a\xi_{n_j}} \prod_{k=1\neq j}^{N} \sum_{\xi_k} |\psi_{\xi_k}(r_k)\rangle \end{aligned}$$

$$\boxed{T_{tot}|\Psi(r_1, r_2, \ldots, r_N)\rangle = \sum_{j=1}^{N} \sum_{\xi_1,\ldots,\xi_b,\ldots,\xi_N} T_{\xi_b\xi_{n_j}} |\psi_{\xi_1}(r_1)\rangle \ldots |\psi_{\xi_b}(r_j)\rangle \ldots |\psi_{\xi_N}(r_N)\rangle} \qquad (4)$$

$T(r_j, \nabla r_j)$ was a one particle operator. To finish off our discussion of Assumption 3, we need to talk about a two particle operator.

Let us now consider the symmetric two particle operator for Coulomb interaction between a pair of electrons, each situated at r_j and r_k respectively.

$$V(r_j - r_k) = \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|r_j - r_k|}$$

We define $V_{\xi_c\xi_d,\xi_a\xi_b}$ and V_{jk} such that :

$$V_{\xi_c\xi_d,\xi_a\xi_b} = \int dr_j^{'} dr_k^{'} \psi^*_{\xi_c}(r_j^{'}) \psi^*_{\xi_d}(r_k^{'}) V(r_j^{'} - r_k^{'}) \psi_{\xi_a}(r_j^{'}) \psi_{\xi_b}(r_k^{'})$$

$$V_{jk} = \sum_{\xi_a\xi_b\xi_c\xi_d} V_{\xi_c\xi_d,\xi_a\xi_b} |\psi_{\xi_c}(r_j)\rangle |\psi_{\xi_d}(r_k)\rangle \langle\psi_{\xi_a}(r_j)| \langle\psi_{\xi_b}(r_k)|$$

Evaulating V_{jk} we obtain :

$$\begin{aligned} V_{jk} &= \sum_{\xi_a\xi_b\xi_c\xi_d} \int dr_j^{'} dr_k^{'} \psi^*_{\xi_c}(r_j^{'}) \psi^*_{\xi_d}(r_k^{'}) V(r_j^{'} - r_k^{'}) \psi_{\xi_a}(r_j^{'}) \psi_{\xi_b}(r_k^{'}) |\psi_{\xi_c}(r_j)\rangle |\psi_{\xi_d}(r_k)\rangle \langle\psi_{\xi_a}(r_j)| \langle\psi_{\xi_b}(r_k)| \\ &= \int dr_j^{'} dr_k^{'} V(r_j^{'} - r_k^{'}) \sum_{\xi_c} \psi^*_{\xi_c}(r_j^{'}) \psi_{\xi_c}(r_j) \sum_{\xi_d} \psi^*_{\xi_d}(r_k^{'}) \psi_{\xi_d}(r_k) \sum_{\xi_a} \psi_{\xi_a}(r_j^{'}) \psi^*_{\xi_a}(r_j) \sum_{\xi_b} \psi_{\xi_b}(r_k^{'}) \psi^*_{\xi_b}(r_k) \\ &= \int dr_j^{'} dr_k^{'} V(r_j^{'} - r_k^{'}) \delta(r_j^{'} - r_j) \delta(r_k^{'} - r_k) \delta(r_j^{'} - r_j) \delta(r_k^{'} - r_k) \end{aligned}$$

$$\boxed{\therefore V_{jk} = V(r_j - r_k)}$$

For N-particle system, we take the symmetric combination of the coordinates, and to do so, we define V_{tot} as :

$$V_{tot} = \sum_{j>k}^{N} V_{jk} = \frac{1}{2} \sum_{j=1, j\neq k}^{N} V_{jk}$$

If it acts on a many-body wave function $\Psi(r_1, r_2, \ldots, r_N)$ then :

$$\begin{aligned} V_{tot} |\Psi(r_1, r_2, \ldots, r_N)\rangle &= V_{tot} \prod_{l=1}^{N} \sum_{\xi_l} |\psi_{\xi_l}(r_l)\rangle \\ &= \frac{1}{2} \sum_{j\neq k}^{N} \sum_{\xi_a\xi_b\xi_c\xi_d} V_{\xi_c\xi_d,\xi_a\xi_b} |\psi_{\xi_c}(r_j)\rangle |\psi_{\xi_d}(r_k)\rangle \langle\psi_{\xi_a}(r_j)| \langle\psi_{\xi_b}(r_k)| \prod_{l=1}^{N} \sum_{\xi_l} |\psi_{\xi_l}(r_l)\rangle \\ &= \frac{1}{2} \sum_{j\neq k}^{N} \sum_{\xi_a\xi_b\xi_c\xi_d} V_{\xi_c\xi_d,\xi_a\xi_b} |\psi_{\xi_c}(r_j)\rangle |\psi_{\xi_d}(r_k)\rangle \langle\psi_{\xi_a}(r_j)| \langle\psi_{\xi_b}(r_k)| \sum_{\xi_j,\xi_k} |\psi_{\xi_j}(r_j)\rangle |\psi_{\xi_k}(r_k)\rangle \\ &\qquad \times \prod_{l=1\neq j\neq k}^{N} \sum_{\xi_l} |\psi_{\xi_l}(r_l)\rangle \end{aligned}$$

$$= \frac{1}{2}\sum_{j\neq k}^{N}\sum_{\xi_a\xi_b\xi_c\xi_d} V_{\xi_c\xi_d,\xi_a\xi_b}|\psi_{\xi_c}(r_j)\rangle|\psi_{\xi_d}(r_k)\rangle \sum_n \langle\psi_{\xi_a}(r_j)|\psi_{\xi_j}(r_j)\rangle \sum_m \langle\psi_{\xi_b}(r_k)|\psi_{\xi_k}(r_k)\rangle$$
$$\times \prod_{l=1\neq j\neq k}^{N}\sum_{\xi_l}|\psi_{\xi_l}(r_l)\rangle$$

$$= \frac{1}{2}\sum_{j\neq k}^{N}\sum_{\xi_a\xi_b\xi_c\xi_d} V_{\xi_c\xi_d,\xi_a\xi_b}|\psi_{\xi_c}(r_j)\rangle\delta_{\xi_a\xi_{n_j}}\delta_{\xi_b\xi_{m_k}} \times \prod_{l=1\neq j\neq k}^{N}\sum_{\xi_l}|\psi_{\xi_l}(r_l)\rangle$$

$$V_{tot}|\Psi(r_1,r_2,\ldots,r_N)\rangle = \frac{1}{2}\sum_{j\neq k}^{N}\sum_{\xi_1,\ldots,\xi_c,\ldots,\xi_d,\ldots,\xi_N} V_{\xi_c\xi_d,\xi_{n_j}\xi_{m_k}}|\psi_{\xi_1}(r_1)\rangle\ldots \times\ldots|\psi_{\xi_c}(r_j)\rangle\ldots|\psi_{\xi_d}(r_k)\rangle\ldots|\psi_{\xi_N}(r_N)\rangle \quad (5)$$

It is also important to note that in the any of the wave functions written above, only the occupied single particle states play a role. So the summation can be dropped if only one quantum number represents occupied state.

$$T_{tot}|\Psi(r_1,r_2,\ldots,r_N)\rangle = \sum_{j=1}^{N}\sum_{\xi_a,\xi_b} T_{\xi_a,\xi_b}\delta_{\xi_a\xi_{n_j}}|\psi_{\xi_{n_1}}(r_1)\rangle\ldots|\psi_{\xi_b}(r_j)\rangle\ldots|\psi_{\xi_{n_N}}(r_N)\rangle \quad (6)$$

$$V_{tot}|\Psi(r_1,r_2\ldots.,r_N)\rangle = \frac{1}{2}\sum_{j\neq k}^{N}\sum_{\xi_a,\xi_b,\xi_c,\xi_d} V_{\xi_c\xi_d,\xi_a\xi_b}\delta_{\xi_a\xi_{n_j}}\delta_{\xi_b\xi_{m_k}}|\psi_{\xi_{n_1}}(r_1)\rangle\ldots \times\ldots|\psi_{\xi_c}(r_j)\rangle\ldots|\psi_{\xi_d}(r_k)\rangle\ldots|\psi_{\xi_{n_N}}(r_N)\rangle \quad (7)$$

iii. Symmetrization ($\hat{S}_+$) and Antisymmetrisation ($\hat{S}_-$) Operators

Let us consider a two particle wave function : $\Psi(r_1, r_2)$
If the particles are bosons, then it must satisfy :

$$\Psi(r_1, r_2) = \Psi(r_2, r_1)$$

If the particles are fermions, then it must satisfy :

$$\Psi(r_1, r_2) = -\Psi(r_2, r_1)$$

We can use the Hartree product as an anstanz to denote the wave function, i.e, let :

$$\Psi(r_1, r_2) = \psi_1(r_1)\psi_2(r_2)$$

But this alone would not satisfy the bosonic symmetry of fermionic anti-symmetry condition. However, using this we can define Ψ such that those conditions would be satisfied.

For **fermions** let us define $\Psi(r_1, r_2)$ as :

$$\Psi(r_1, r_2) = \frac{1}{\sqrt{2}} \{\psi_1(r_1)\psi_2(r_2) - \psi_1(r_2)\psi_2(r_1)\} = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_1(r_1) & \psi_1(r_2) \\ \psi_2(r_1) & \psi_2(r_2) \end{vmatrix}$$

Generalising for any number of fermions :

$$\Psi(r_1, r_2, \ldots, r_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(r_1) & \psi_1(r_2) & \ldots & \psi_1(r_N) \\ \psi_2(r_1) & \psi_2(r_2) & \ldots & \psi_2(r_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_N(r_1) & \psi_N(r_2) & \ldots & \psi_N(r_N) \end{vmatrix}$$

Similarly, for **bosons**, we can define $\Psi(r_1, r_2)$ as :

$$\Psi(r_1, r_2) = \frac{1}{\sqrt{2}} \{\psi_1(r_1)\psi_2(r_2) + \psi_1(r_2)\psi_2(r_1)\} = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_1(r_1) & \psi_1(r_2) \\ \psi_2(r_1) & \psi_2(r_2) \end{vmatrix}_+$$

This is a signless determinant, also called a permanant. Generalising for any number of bosons :

$$\Psi(r_1, r_2, \ldots, r_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(r_1) & \psi_1(r_2) & \ldots & \psi_1(r_N) \\ \psi_2(r_1) & \psi_2(r_2) & \ldots & \psi_2(r_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_N(r_1) & \psi_N(r_2) & \ldots & \psi_N(r_N) \end{vmatrix}_+$$

These are called Slater's determinant.

$$\hat{S}_\pm = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(r_1) & \psi_1(r_2) & \ldots & \psi_1(r_N) \\ \psi_2(r_1) & \psi_2(r_2) & \ldots & \psi_2(r_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_N(r_1) & \psi_N(r_2) & \ldots & \psi_N(r_N) \end{vmatrix}_\pm$$

$\hat{S}_+$ is a permanant, and called Bosonic Symmetrisation Operator. $\hat{S}_-$ is a determinant, and is called Fermionic Anti-Symmetrisation Operator.

III. Second Quantisation

Also known as Occupation Number Representation, it is a formalism used to represent and analyse quantum many-body systems. The quantum many-body states are represented in the Fock state basis and creation and annihilation operators are used to construct and study the Fock states.

i. Occupation Number Representation

First we have to choose any ordered and complete single particle basis $\{|\xi_1\rangle|\xi_2\rangle, \ldots, |\xi_n\rangle\}$.
The basis state for a N particle system in the occupation number representation is obtained by writing down the occupation numbers of each basis state :

$$|n_{\xi_1}, n_{\xi_2}, n_{\xi_3}, \ldots\rangle; \quad \sum_j n_{\xi_j} = N$$

n_{ξ_j} represents the number of particles occupying state ξ_j.
We define occupation number operators, $\hat{n}_{\xi_j}$, which have basis states $|n_{\xi_j}\rangle$ as eigen states, and n_{ξ_j} as eigen values.

$$\hat{n}_{\xi_j}|n_{\xi_j}\rangle = n_{\xi_j}|n_{\xi_j}\rangle$$

We can write from our previous discussion on bosons and fermions that :

$$n_{\xi_j} = \begin{cases} 0, \quad 1 & \text{(fermions)} \\ 0, \quad 1, \quad 2, \quad \ldots & \text{(bosons)} \end{cases}$$

The space spanned by the occupation number basis is the Fock space $\mathcal{F}$.

$$\mathcal{F} = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \mathcal{F}_2 \oplus \cdots$$

The states containing different number of particles are defined to be orthogonal due to the direct sum.

ii. Bosonic Creation and Annihilation Operators

Creation operator $b^\dagger_{\xi_j}$ raises the occupation number in the state $|\xi_j\rangle$ by 1.

$$b^\dagger_{\xi_j}|\ldots, n_{\xi_{j-1}}, n_{\xi_j}, n_{\xi_{j+1}}, \ldots\rangle = B_+(n_{\xi_j})|\ldots, n_{\xi_{j-1}}, n_{\xi_j}+1, n_{\xi_{j+1}}, \ldots\rangle$$

$B_+(n_{\xi_j})$ is the normalization constant.
If we take the inner product with $\langle n_{\xi_j}+1|$, term by term, then $\langle n_{\xi_j}+1|b^\dagger_{\xi_j}|n_{\xi_j}\rangle$ is the only non-zero term.

$$\langle n_{\xi_j}+1|b^\dagger_{\xi_j}|n_{\xi_j}\rangle = 1$$

Taking complex conjugate of the above term :

$$\begin{aligned} \langle n_{\xi_j}+1|b^\dagger_{\xi_j}|n_{\xi_j}\rangle^* &= 1 \\ \implies \langle n_{\xi_j}|(b^\dagger_{\xi_j})^\dagger|n_{\xi_j}+1\rangle &= 1 \end{aligned}$$

Annihilation Operator b_{ξ_j} reduces the occupation number in the state $|\xi_j\rangle$ by 1.

$$b_{\xi_j}|\ldots, n_{\xi_{j-1}}, n_{\xi_j}, n_{\xi_{j+1}}, \ldots\rangle = B_-(n_{\xi_j})|\ldots, n_{\xi_{j-1}}, n_{\xi_j} - 1, n_{\xi_{j+1}}, \ldots\rangle$$

$B_-(n_{\xi_j})$ is the normalization constant.
As an unoccupied state cannot be emptied further, we can set such an operation to be 0.

$$b_{\xi_j}|\ldots, 0, \ldots\rangle = 0; \quad \text{i.e., } B_-(0) = 0$$

As bosons are symmetric in the single particle basis state, so :

$$|\ldots, n_{\xi_j} \pm 1, \ldots, n_{\xi_k} \pm 1 \ldots\rangle = |\ldots n_{\xi_k} \pm 1, \ldots, n_{\xi_j} \pm 1 \ldots\rangle$$

Also as an added consequence of the symmetric nature, the order of action of creation and annihilation operators ***on different states*** does not make any difference.If creation and annihilation operators act on the same state, the results do not commute. For eg :

$$\begin{aligned} b_\xi b_\xi^\dagger|0\rangle &= b_\xi|1\rangle = |0\rangle \\ b_\xi^\dagger b_\xi|0\rangle &= 0 \\ (b_\xi b_\xi^\dagger - b_\xi^\dagger b_\xi)|0\rangle &= |0\rangle \end{aligned}$$

Using the above facts, we can say that :

$$\boxed{\begin{aligned} [b_{\xi_j}^\dagger, b_{\xi_k}^\dagger] &= 0 \quad (8) \\ [b_{\xi_j}, b_{\xi_k}] &= 0 \quad (9) \\ [b_{\xi_j}, b_{\xi_k}^\dagger] &= \delta_{\xi_j,\xi_k} \quad (10) \end{aligned}}$$

We must also keep in mind that $b_\xi^\dagger$ and b_ξ are not Hermitian, so they do not represent any measurable quantities. They simply act to add or remove bosonic particles from a particular state. Their product $b_\xi^\dagger b_\xi$ however, is Hermitian, and represents some measurable physical quantity. Infact, $b_\xi^\dagger b_\xi$ is actually the occupation number operator $\hat{n}_\xi$ for bosons of any state $|\xi\rangle$. We can conclude this very significant result from the eigen states and eigen values of $b_\xi^\dagger b_\xi$.

a. Showing $b_\xi^\dagger b_\xi = \hat{n}_\xi$

Let us consider any state $|\phi\rangle$. We observe that :

$$\langle\phi|b_\xi^\dagger b_\xi|\phi\rangle = \{b_\xi|\phi\rangle\}^\dagger \{b_\xi|\phi\rangle\} = ||b_\xi|\phi\rangle||^2 \geq 0$$

Taking into account the above condition and assuming $|\phi_\lambda\rangle$ to be some eigen state of $b_\xi^\dagger b_\xi$ with eigen value λ, we can write :

$$b_\xi^\dagger b_\xi|\phi_\lambda\rangle = \lambda|\phi_\lambda\rangle \ ; \quad \lambda \geq 0$$

Let λ_0 be any particular eigen value and $|\phi_{\lambda_0}\rangle$. Let us consider the action of $b_\xi^\dagger b_\xi$ on $b_\xi|\phi_{\lambda_0}\rangle$:

$$\begin{aligned}
(b_\xi^\dagger b_\xi)b_\xi|\phi_{\lambda_0}\rangle &= (b_\xi b_\xi^\dagger - 1)b_\xi|\phi_{\lambda_0}\rangle \qquad \text{(from Equation 10)} \\
&= (b_\xi b_\xi^\dagger b_\xi - b_\xi)|\phi_{\lambda_0}\rangle \\
&= b_\xi(b_\xi^\dagger b_\xi - 1)|\phi_{\lambda_0}\rangle \\
&= b_\xi\left\{\lambda_0|\phi_{\lambda_0}\rangle - |\phi_{\lambda_0}\rangle\right\} \\
&= b_\xi(\lambda_0 - 1)|\phi_{\lambda_0}\rangle \\
\therefore (b_\xi^\dagger b_\xi)b_\xi|\phi_{\lambda_0}\rangle &= (\lambda_0 - 1)b_\xi|\phi_{\lambda_0}\rangle
\end{aligned}$$

Thus, b_ξ is also an eigen state of $b_\xi^\dagger b_\xi$, but with the eigen value reduced by 1, to $(\lambda_0 - 1)$. This can go on until a negative value is hit, as negative values are not allowed. So, $\lambda = 0, 1, 2, \ldots$ Writing, $|\phi_\lambda\rangle = |n_\xi\rangle$, with n_ξ as eigen values, we see that :

$$\begin{aligned}
(b_\xi^\dagger b_\xi)b_\xi|n_\xi\rangle = (n_\xi - 1)b_\xi|n_\xi\rangle = B_-(n_\xi)(n_\xi - 1)|n_\xi\rangle \quad &\text{and} \\
b_\xi^\dagger b_\xi|n_\xi\rangle = n_\xi|n_\xi\rangle &
\end{aligned}$$

Comparing these with the action of operator $\hat{n}_\xi$, we can immediately see that $b_\xi^\dagger b_\xi = n_\xi$.

b. Normalization constants of $b_\xi^\dagger$ and b_ξ

Computing the normalization constants of $b_\xi^\dagger$ and b_ξ using this information :

$$\begin{aligned}
||b_\xi|n_\xi\rangle||^2 &= \langle n_\xi|b_\xi^\dagger b_\xi|n_\xi\rangle = B_-^*(n_\xi)B_-(n_\xi)\langle n_\xi|n_\xi\rangle = n_\xi\langle n_\xi|n_\xi\rangle \\
\implies |B_-(n_\xi)|^2 &= n_\xi
\end{aligned}$$

$$\therefore \boxed{B_-(n_\xi) = \sqrt{n_\xi}}$$

$$\begin{aligned}
||b_\xi^\dagger|n_\xi\rangle||^2 &= \langle n_\xi|b_\xi b_\xi^\dagger|n_\xi\rangle = B_+^*(n_\xi)B_+(n_\xi)\langle n_\xi|n_\xi\rangle \\
&= \langle n_\xi|(b_\xi^\dagger b_\xi + 1)|n_\xi\rangle = (n_x i + 1)\langle n_\xi|n_\xi\rangle \\
\implies |B_+(n_\xi)|^2 &= n_\xi + 1
\end{aligned}$$

$$\therefore \boxed{B_+(n_\xi) = \sqrt{n_\xi + 1}}$$

Using all the above information we can derive two interesting properties of $b_\xi^\dagger b_\xi$, i.e., $[b_\xi^\dagger b_\xi, b_\xi] = -b_\xi$ and $[b_\xi^\dagger b_\xi, b_\xi^\dagger] = b_\xi^\dagger$

c. $[b_\xi^\dagger b_\xi, b_\xi] = -b_\xi$

To verify this relation, we need to study the action of this commutator on $|n_\xi\rangle$:

$$\begin{aligned}
[b_\xi^\dagger b_\xi, b_\xi]|n_\xi\rangle &= b_\xi^\dagger b_\xi b_\xi|n_\xi\rangle - b_\xi b_\xi^\dagger b_\xi|n_\xi\rangle \\
&= b_\xi^\dagger b_\xi B_-(n_\xi)|n_\xi - 1\rangle - b_\xi b_\xi^\dagger B_-(n_\xi)|n_\xi - 1\rangle \\
&= b^\dagger B_-(n_\xi - 1)B_-(n_\xi)|n_\xi - 2\rangle - b_\xi B_+(n_\xi - 1)B_-(n_\xi)|n_\xi\rangle \\
&= B_+(n_\xi - 2)B_-(n_\xi - 1)B_-(n_\xi)|n_\xi - 1\rangle - B_-(n_\xi)B_+(n_\xi - 1)B_-(n_\xi)|n_\xi - 1\rangle
\end{aligned}$$

Using the normalization constants calculated in the previous sub-subsection, we can write :

$$\begin{aligned}
&= \left(\sqrt{n_\xi - 1}\sqrt{n_\xi - 1}\sqrt{n_\xi} - \sqrt{n_\xi}\sqrt{n_\xi}\sqrt{n_\xi}\right)|n_\xi - 1\rangle \\
&= \sqrt{n_\xi}\,(n_\xi - 1 - n_\xi)\,|n_\xi - 1\rangle \\
&= \sqrt{n_\xi}(-1)|n_\xi - 1\rangle \\
&= (-1)B_-(n_\xi)|n_\xi - 1\rangle \\
&= (-1)b_\xi|n_\xi\rangle
\end{aligned}$$

$$\therefore \boxed{[b_\xi^\dagger b_\xi, b_\xi] = -b_\xi}$$

d. $[b_\xi^\dagger b_\xi, b_\xi^\dagger] = b_\xi^\dagger$

To verify this relation, we need to study the action of this commutator on $|n_\xi\rangle$:

$$\begin{aligned}
[b_\xi^\dagger b_\xi, b_\xi^\dagger]|n_\xi\rangle &= b_\xi^\dagger b_\xi b_\xi^\dagger|n_\xi\rangle - b_\xi^\dagger b_\xi^\dagger b_\xi|n_\xi\rangle \\
&= b_\xi^\dagger b_\xi B_+(n_\xi)|n_\xi + 1\rangle - b_\xi^\dagger b_\xi^\dagger B_-(n_\xi)|n_\xi - 1\rangle \\
&= b_\xi^\dagger B_-(n_\xi + 1)B_+(n_\xi)|n_\xi\rangle - b^\dagger B_+(n_\xi - 1)B_-(n_\xi)|n_\xi\rangle \\
&= B_+(n_\xi)\left(B_-(n_\xi + 1)B_+(n_\xi) - B_+(n_\xi - 1)B_-(n_\xi)\right)|n_\xi + 1\rangle
\end{aligned}$$

Using the normalization constants calculated in the previous sub-subsection, we can write :

$$\begin{aligned}
&= \sqrt{n_\xi + 1}\left(\sqrt{n_\xi + 1}\sqrt{n_\xi + 1} - \sqrt{n_\xi}\sqrt{n_\xi}\right)|n_\xi + 1\rangle \\
&= \sqrt{n_\xi + 1}\,(n_\xi + 1 - n_\xi)\,|n_\xi + 1\rangle \\
&= \sqrt{n_\xi + 1}|n_\xi + 1\rangle \\
&= b_\xi^\dagger|n_\xi\rangle
\end{aligned}$$

$$\therefore \boxed{[b_\xi^\dagger b_\xi, b_\xi^\dagger] = b_\xi^\dagger}$$

Now, we can write the first quantised basis states in second quantised basis states :

$$\boxed{\hat{S}_+|\psi_{\xi_{n_1}}(r_1)\rangle|\psi_{\xi_{n_2}}(r_2)\rangle \ldots |\psi_{\xi_{n_N}}(r_N)\rangle = b_{\xi_{n_1}}^\dagger b_{\xi_{n_2}}^\dagger \ldots b_{\xi_{n_N}}^\dagger|0\rangle} \tag{11}$$

iii. Fermionic Creation and Annihilation Operators

Creation operator $c^\dagger_{\xi_j}$ raises the occupation number in the state $|\xi_j\rangle$ by 1.

$$c^\dagger_{\xi_j}|\ldots, n_{\xi_{j-1}}, n_{\xi_j}, n_{\xi_{j+1}}, \ldots\rangle = C_+(n_{\xi_j})|\ldots, n_{\xi_{j-1}}, n_{\xi_j}+1, n_{\xi_{j+1}}, \ldots\rangle$$

$C_+(n_{\xi_j})$ is the normalization constant.
If we take the inner product with $\langle n_{\xi_j}+1|$, term by term, then $\langle n_{\xi_j}+1|c^\dagger_{\xi_j}|n_{\xi_j}\rangle$ is the only non-zero term.

$$\langle n_{\xi_j}+1|c^\dagger_{\xi_j}|n_{\xi_j}\rangle = 1$$

Taking complex conjugate of the above term :

$$\begin{aligned} &\langle n_{\xi_j}+1|c^\dagger_{\xi_j}|n_{\xi_j}\rangle^* = 1 \\ \implies &\langle n_{\xi_j}|(c^\dagger_{\xi_j})^\dagger|n_{\xi_j}+1\rangle = 1 \end{aligned}$$

Annihilation Operator c_{ξ_j} reduces the occupation number in the state $|\xi_j\rangle$ by 1.

$$c_{\xi_j}|\ldots, n_{\xi_{j-1}}, n_{\xi_j}, n_{\xi_{j+1}}, \ldots\rangle = C_-(n_{\xi_j})|\ldots, n_{\xi_{j-1}}, n_{\xi_j}-1, n_{\xi_{j+1}}, \ldots\rangle$$

$C_-(n_{\xi_j})$ is the normalization constant.
As an unoccupied state cannot be emptied further, we can set such an operation to be 0.

$$c_{\xi_j}|\ldots, 0, \ldots\rangle = 0; \quad \text{i.e., } C_-(0) = 0$$

Also, due to anti-symmetric nature of fermions, only two possible states are allowed : $|0\rangle$ and $|1\rangle$. Adding any particle to $|1\rangle$ is also physically impossible, so :

$$c^\dagger_{\xi_j}|\ldots, 1, \ldots\rangle = 0; \quad \text{i.e., } C_+(1) = 0$$

As fermions are anti-symmetric in the single particle basis state, so :

$$|\ldots, n_{\xi_j}\pm 1, \ldots, n_{\xi_k}\pm 1\ldots\rangle = -|\ldots n_{\xi_k}\pm 1, \ldots, n_{\xi_j}\pm 1\ldots\rangle$$

Also as an added consequence of the anti-symmetric nature, the order of action of creation and annihilation operators ***on different states*** is equivalent to switching the position of two fermions.If creation and annihilation operators act on the same state, the results do not anti-commute. For eg :

$$\begin{aligned} c_\xi c^\dagger_\xi|0\rangle &= c_\xi|1\rangle = |0\rangle \\ c^\dagger_\xi c_\xi|0\rangle &= 0 \\ (c_\xi c^\dagger_\xi - c^\dagger_\xi c_\xi)|0\rangle &= |0\rangle \end{aligned}$$

Using the above facts, we can say that :

$$\boxed{\begin{aligned}\{c^\dagger_{\xi_j}, c^\dagger_{\xi_k}\} &= 0 \quad (12)\\ \{c_{\xi_j}, c_{\xi_k}\} &= 0 \quad (13)\\ \{c_{\xi_j}, c^\dagger_{\xi_k}\} &= \delta_{\xi_j,\xi_k} \quad (14)\end{aligned}}$$

Just like bosonic creation and annihilation operators, $c^\dagger_\xi$ and c_ξ are not Hermitian. so they do not represent any measurable quantities. They simply act to add or remove fermionic particles from a particular state. Their product $c^\dagger_\xi c_\xi$ however, is Hermitian, and represents some measurable physical quantity. Like the bosonic case, it is actually the occupation number operator $\hat{c}_\xi$ for fermions of any state $|\xi\rangle$. We can conclude this very significant result, like before, from the eigen states and eigen values of $c^\dagger_\xi c_\xi$.

a. Normalization constants of $c^\dagger_\xi$ and c_ξ

Due to the anti-symmetric nature of fermions, there cannot be more than one particle in any state. So, $|0\rangle$ and $|1\rangle$ are the only two allowed states. So,

$$\begin{aligned}c_\xi|0\rangle &= 0; \quad C_-(0) = 0\\ c_\xi|1\rangle &= C_-(1)|0\rangle\\ c^\dagger_\xi|1\rangle &= 0; \quad C_+(1) = 0\\ c^\dagger_\xi|0\rangle &= C_+(0)|1\rangle\end{aligned}$$

Using the above relations we can see :

$$\begin{aligned}\langle 0|c_\xi|1\rangle &= \langle 1|c^\dagger_\xi|0\rangle\\ \implies C_-(1) &= C_+(0)^*\end{aligned}$$

We have the freedom to demand :

$$\boxed{C_-(1) = C_+(0) = 1}$$

b. Showing $c^\dagger_\xi c_\xi = \hat{n}_\xi$

Studying the action of $c^\dagger_\xi c_\xi$ on the two allowed $|n_\xi\rangle$: $|0\rangle$ and $|1\rangle$

$$\begin{aligned}c^\dagger_\xi c_\xi|0\rangle &= 0\\ c^\dagger_\xi c_\xi|1\rangle &= c^\dagger_\xi|0\rangle = |1\rangle\end{aligned}$$

Comparing it with $\hat{n}_\xi$:

$$c^\dagger_\xi c_\xi|n_\xi\rangle = \hat{n}_\xi|n_\xi\rangle; \quad n_\xi = 0, 1$$

Using all the above relations we can derive two interesting properties of $c_\xi^\dagger c_\xi$, i.e., $[c_\xi^\dagger c_\xi, c_\xi] = -c_\xi$ and $[c_\xi^\dagger c_\xi, c_\xi^\dagger] = c_\xi^\dagger$

c. $[c_\xi^\dagger c_\xi, c_\xi] = -c_\xi$

To verify this relation, we need to study the action of this commutator on $|1\rangle$:

$$\begin{aligned}[c_\xi^\dagger c_\xi, c_\xi]|1\rangle &= c_\xi^\dagger c_\xi c_\xi|1\rangle - c_\xi c_\xi^\dagger c_\xi|1\rangle \\ &= c_\xi^\dagger c_\xi|0\rangle - c_\xi c_\xi^\dagger|0\rangle \\ &= 0 - c_\xi|1\rangle \\ \therefore \boxed{[c_\xi^\dagger c_\xi, c_\xi] = -c_\xi}\end{aligned}$$

d. $[c_\xi^\dagger c_\xi, c_\xi^\dagger] = c_\xi^\dagger$

To verify this relation, we need to study the action of this commutator on $|0\rangle$:

$$\begin{aligned}[c_\xi^\dagger c_\xi, c_\xi]|0\rangle &= c_\xi^\dagger c_\xi c_\xi^\dagger|0\rangle - c_\xi^\dagger c_\xi^\dagger c_\xi|0\rangle \\ &= c_\xi^\dagger c_\xi|1\rangle - 0 \\ &= c_\xi^\dagger|0\rangle \\ \therefore \boxed{[c_\xi^\dagger c_\xi, c_\xi^\dagger] = c_\xi^\dagger}\end{aligned}$$

Now, we can write the first quantised basis states in second quantised basis states :

$$\boxed{\hat{S}_-|\psi_{\xi_{n_1}}(r_1)\rangle|\psi_{\xi_{n_2}}(r_2)\rangle\ldots|\psi_{\xi_{n_N}}(r_N)\rangle = c_{\xi_{n_1}}^\dagger c_{\xi_{n_2}}^\dagger \ldots c_{\xi_{n_N}}^\dagger|0\rangle} \tag{15}$$

iv. General form of Second quantisation operators

In second quantisation we can represent all operators in terms of creation and annihilation operators.
Let us consider T_{tot} acting on a bosonic N-particle system :

$$\begin{aligned}\hat{S}_+|\psi_{\xi_{n_1}}(r_1)\rangle|\psi_{\xi_{n_2}}(r_2)\rangle\ldots|\psi_{\xi_{n_N}}\rangle &= b_{\xi_{n_1}}^\dagger b_{\xi_{n_2}}^\dagger \ldots b_{\xi_{n_N}}^\dagger|0\rangle \\ T_{tot}|\psi_{\xi_{n_1}}(r_1)\rangle|\psi_{\xi_{n_2}}(r_2)\rangle\ldots|\psi_{\xi_{n_N}}\rangle &= \sum_{j=1}^{N}\sum_{\xi_a\xi_b} T_{\xi_a\xi_b}\delta_{\xi_a\xi_{n_j}}|\psi_{\xi_{n_1}}(r_1)\rangle\ldots|\psi_{\xi_b}(r_j)\rangle\ldots|\psi_{\xi_{n_N}}(r_N)\rangle\end{aligned}$$

So,

$$T_{tot}b_{\xi_{n_1}}^\dagger b_{\xi_{n_2}}^\dagger \ldots b_{\xi_{n_N}}^\dagger|0\rangle = \sum_{\xi_a\xi_b} T_{\xi_a\xi_b}\sum_{j=1}^{N}\delta_{\xi_a\xi_{n_j}} b_{\xi_{n_1}}^\dagger b_{\xi_{n_2}}^\dagger \ldots b_{\xi_b}^\dagger \ldots b_{\xi_{n_N}}^\dagger|0\rangle$$

The term $b^\dagger_{\xi_b}$ sits in the position of $b^\dagger_{\xi_{n_j}}$.

The state ξ_a my appear p times in the LHS, $p > 0$. In the RHS, it appears as $b^\dagger_{\xi_b}\left(b^\dagger_{\xi_a}\right)^{p-1}$.

$$\text{So, } \left(b^\dagger_{\xi_a}\right)^p|0\rangle = b^\dagger_{\xi_b}\left(b^\dagger_{\xi_a}\right)^{p-1}|0\rangle$$

$$\begin{aligned}
\text{Let } b^\dagger_{\xi_a} &\equiv b^\dagger_\xi \\
\left(b^\dagger_\xi\right)^{p-1}|0\rangle &= \sqrt{(p-1)!}|p-1\rangle \\
b^\dagger_\xi\sqrt{(p-1)!}|p-1\rangle &= \sqrt{(p-1)!}\sqrt{p}|p\rangle \\
b_\xi\sqrt{(p-1)!}\sqrt{p}|p\rangle &= p\sqrt{(p-1)!}|p-1\rangle \\
\text{Thus, } \left(\frac{1}{p}b_\xi b^\dagger_\xi\right)\left(b^\dagger_\xi\right)^{p-1}|0\rangle &= \left(b^\dagger_\xi\right)^{p-1}|0\rangle
\end{aligned}$$

$$\begin{aligned}
\text{So, } b^\dagger_{\xi-b}\left(b^\dagger_\xi\right)^{p-1}|0\rangle &= b^\dagger_{\xi_b}\left(\frac{1}{p}b_\xi b^\dagger_{\xi_b}\right)\left(\frac{1}{p}b_\xi b^\dagger_\xi\right)\left(b^\dagger_\xi\right)^{p-1}|0\rangle \\
&= \left(\frac{1}{p}b^\dagger_{\xi_b}b_\xi\right)\left(b^\dagger_\xi\right)^p|0\rangle
\end{aligned}$$

The sum over j with $\delta_{\xi_a\xi_{n_j}}$ yields p identical contributions canceling $\frac{1}{p}$:

$$T_{tot}\left[b^\dagger_{\xi_{n_1}}b^\dagger_{\xi_{n_2}}\ldots b^\dagger_{\xi_{n_N}}|0\rangle\right] = \sum_{\xi_a\xi_b}T_{\xi_a\xi_b}b^\dagger_{\xi_b}b_{\xi_a}\left[b^\dagger_{\xi_{n_1}}b^\dagger_{\xi_{n_2}}\ldots b^\dagger_{\xi_{n_N}}|0\rangle\right]$$

We can do the same for two particle operators.

We can generalize this for bosons and fermions, if we take appropriate care regarding the signs appearing, and write :

$$\boxed{\begin{aligned}
T_{tot} &= \sum_{\xi_i\xi_j}T_{\xi_i\xi_j}a^\dagger_{\xi_i}a_{\xi_j} \qquad (16)\\
V_{tot} &= \frac{1}{2}\sum_{\xi_i\xi_j\xi_k\xi_l}V_{\xi_i\xi_j,\xi_k\xi_l}a^\dagger_{\xi_i}a^\dagger_{\xi_j}a_{\xi_l}a_{\xi_k} \qquad (17)
\end{aligned}}$$

$a^\dagger_\xi$ is the bosonicor fermionic creation operator.

a_ξ is the bosonic or fermionic annihilator operator.

The order of the indices is very important in fermionic two particle operators.

$$\begin{aligned}
|0\rangle &= a_{\xi_l}a_{\xi_k}|\xi_k\xi_l\rangle \\
|\xi_i\xi_j\rangle &= a^\dagger_{\xi_i}a^\dagger_{\xi_j}|0\rangle
\end{aligned}$$

These relations take care of the symmetry or anti-symmetry properties of the operators.

v. Change of Basis

Let $\left\{|\psi_{\xi_1}\rangle|\psi_{\xi_2}\rangle\dots\right\}$ and $\left\{|\tilde{\psi}_{\mu_1}\rangle|\tilde{\psi}_{\mu_2}\rangle\dots\right\}$ be two different complete and ordered single particle basis sets.

Basic transformation law for single particle states tells us that :

$$|\tilde{\psi}_\mu\rangle = \sum_\xi |\psi_\xi\rangle\langle\psi_\xi|\tilde{\psi}_\mu\rangle = \sum_\xi \langle\tilde{\psi}_\mu|\psi_\xi\rangle^*|\psi_\xi\rangle$$

If $\tilde{a}^\dagger_\mu|0\rangle = |\tilde{\psi}_\mu\rangle$, and $a^\dagger_\xi|0\rangle = |\psi_\xi\rangle$, then the above equation can be rewritten as :

$$\tilde{a}^\dagger_\mu|0\rangle = \sum_\xi \langle\tilde{\psi}_\mu|\psi_\xi\rangle^* a^\dagger_\xi|0\rangle$$

Thus we can write the transformation rules for creation and annihilation operators as :

$$\tilde{a}^\dagger_\mu = \sum_\xi \langle\tilde{\psi}_\mu|\psi_\xi\rangle^* a^\dagger_\xi$$
$$\tilde{a}_\mu = \sum_\xi \langle\tilde{\psi}_\mu|\psi_\xi\rangle a_\xi$$

Generalizing for N-particles :

$$\tilde{a}^\dagger_{\mu_{n_1}}\tilde{a}^\dagger_{\mu_{n_2}}\dots\tilde{a}^\dagger_{\mu_{n_N}}|0\rangle = \left(\sum_{\xi_{n_1}}\langle\tilde{\psi}_{\xi_{n_1}}|\psi_{\xi_{n_1}}\rangle^* a^\dagger_{\xi_{n_1}}\right)\dots\left(\sum_{\xi_{n_N}}\langle\tilde{\psi}_{\mu_{n_N}}|\psi_{\xi_{n_N}}\rangle^* a^\dagger_{\xi_{n_N}}\right)|0\rangle$$

Additionally. this transformation has two useful properties :

a. Preserves the bosonic and fermionic particle statistics

Taking the commutator/anti-commutator relation of $\tilde{a}_{\mu_1}$ and $\tilde{a}^\dagger_{\mu_2}$:

$$\begin{aligned}
\left[\tilde{a}_{\mu_1}, \tilde{a}^\dagger_{\mu_2}\right]_\pm &= \tilde{a}_{\mu_1}\tilde{a}^\dagger_{\mu_2} \pm \tilde{a}^\dagger_{\mu_2}\tilde{a}_{\mu_1} \\
&= \sum_{\xi_i\xi_j}\langle\tilde{\psi}_{\mu_1}|\psi_{\xi_j}\rangle\langle\tilde{\psi}_{\mu_2}|\psi_{\xi_k}\rangle^* a^\dagger_{\xi_j}a^\dagger_{\xi_k} \pm \sum_{\xi_j\xi_k}\langle\tilde{\psi}_{\mu_2}|\psi_{\xi_k}\rangle^*\langle\tilde{\psi}_{\mu_1}|\psi_{\xi_j}\rangle a^\dagger_{\xi_k}a_{\xi_j} \\
&= \sum_{\xi_j\xi_k}\langle\tilde{\psi}_{\mu_1}|\psi_{\xi_j}\rangle\langle\tilde{\psi}_{\mu_2}|\psi_{\xi_k}\rangle^*\left(a_{\xi_j}a^\dagger_{\xi_k} \pm a^\dagger_{\xi_k}a_{\xi_j}\right) \\
&= \sum_{\xi_j\xi_k}\langle\tilde{\psi}_{\mu_1}|\psi_{\xi_j}\rangle\langle\tilde{\psi}_{\mu_2}|\psi_{\xi_k}\rangle^*\left[a_{\xi_j}, a^\dagger_{\xi_k}\right]
\end{aligned}$$

We know from before $[a_{\xi_j}, a^\dagger_{\xi_k}] = \delta_{\xi_j\xi_k}$:

$$\begin{aligned}
&= \sum_{\xi_j\xi_k}\langle\tilde{\psi}_{\mu_1}|\psi_{\xi_j}\rangle\langle\tilde{\psi}_{\mu_2}|\psi_{\xi_k}\rangle^*\delta_{\xi_j\xi_k} \\
&= \sum_{\xi_j}\langle\tilde{\psi}_{\mu_1}|\psi_{\xi_j}\langle\rangle\tilde{\psi}_{\mu_2}|\psi_{\xi_j}\rangle^*
\end{aligned}$$

$$= \sum_{\xi_j} \langle \tilde{\psi}_{\mu_1} | \psi_{\xi_j} \rangle \langle \psi_{\xi_j} | \tilde{\psi}_{\mu_2} \rangle$$

We know that $\sum_{\xi_j} |\psi_{\xi_j}\rangle\langle\psi_{\xi_j}|$ is the identity operator. Thus :

$$\therefore \left[\tilde{a}_{\mu_1}, \tilde{a}^\dagger_{\mu_2}\right]_\pm = \langle \tilde{\psi}_{\mu_1} | \tilde{\psi}_{\mu_2} = \delta_{\mu_1 \mu_2}$$

b. Leaves the total number of particles unchanged

Taking $a^\dagger_\mu a_\mu$ and summing over μ :

$$\begin{aligned}
\sum_\mu a^\dagger_\mu a_\mu &= \sum_\mu \sum_{\xi_j \xi_k} \langle \tilde{\psi}_\mu | \psi_{\xi_j} \rangle^* \langle \tilde{\psi}_\mu | \psi_{\xi_k} \rangle a^\dagger_{\xi_j} a_{\xi_k} \\
&= \sum_\mu \sum_{\xi_j \xi_k} \langle \psi_{\xi_j} | \tilde{\psi}_\mu \rangle \langle \tilde{\psi}_\mu | \psi_{\xi_k} \rangle a^\dagger_{\xi_j} a_{\xi_k} \\
&= \sum_{\xi_j \xi_k} \langle \psi_{\xi_j} | \psi_{\xi_k} \langle a^\dagger_{\xi_j} a_{\xi_k} \\
&= \sum_{\xi_j \xi_k} \delta_{\xi_j \xi_k} a^\dagger_{\xi_j} a_{\xi_k} \\
\therefore \sum_\mu a^\dagger_\mu a_\mu &= \sum_{\xi_j} a^\dagger_{\xi_j} a_{\xi_j}
\end{aligned}$$

vi. Quantum Field Operators

If we let $\left\{|\tilde{\psi}_\mu\rangle\right\}$ be the continuous set of position kets $\{|\boldsymbol{r}\rangle\}$; and represent $a^\dagger_\mu$ by $\Psi^\dagger(\boldsymbol{r})$ (ignoring spin index), then :

$$\begin{aligned}
\Psi^\dagger(\boldsymbol{r}) &\equiv \sum_\xi \langle \boldsymbol{r} | \psi_\xi \rangle^* a^\dagger_\xi = \sum_\xi \psi^*_\xi(\boldsymbol{r}) a^\dagger_\xi \\
\Psi(\boldsymbol{r}) &\equiv \sum_\xi \langle \boldsymbol{r} | \psi_\xi \rangle a_\xi = \sum_\xi \psi_\xi(\boldsymbol{r}) a_\xi
\end{aligned}$$

$\Psi^\dagger(\boldsymbol{r})$ is the sum of all possible ways to add a particle to the system at position $\boldsymbol{r}$ through any of the basis states $\psi_\xi(\boldsymbol{r})$. $\Psi^\dagger(\boldsymbol{r})$ and $\Psi(\boldsymbol{r})$ are called quantum field operators.

$$\begin{aligned}
\left[\Psi(\boldsymbol{r_1}), \Psi^\dagger(\boldsymbol{r_2})\right] &= \delta(\boldsymbol{r_1} - \boldsymbol{r_2}) \qquad \text{Boson fields} \\
\left\{\Psi(\boldsymbol{r_1}), \Psi^\dagger(\boldsymbol{r_2})\right\} &= \delta(\boldsymbol{r_1} - \boldsymbol{r_2}) \qquad \text{Fermionic fields}
\end{aligned}$$

Thus in second quantisation the wave functions essentially become an operator.

IV. BCS Theory of Superconductivity

Superconductivity is a set of physical properties observed in certain materials below some specific critical temperature T_c, the two most fundamental being :

(i) **Perfect DC conductivity ($\boldsymbol{\sigma = \infty}$) below $\boldsymbol{T_c}$** : The transition occurs from a finite resistivity ρ_n above T_c to $\rho = 0$ below T_c.

(ii) **Perfect diamagnetism below $\boldsymbol{T_c}$** (Meissner's Effect) : The change occurs from a small positive paramagnetic value above T_c to $\chi = -1$ (diamagnetic value) below T_c.

The DC currents is superconductors, also known as as supercurrents, can ideally run without any observable loss for years, perhaps for more than 10^6 years.
Superconductivity is a pure quantum physics phenomenon on a macroscopic scale.

BCS Theory of Superconductivity is the first microscopic theory of the phenomenon of superconductivity. It depends on an earlier work of Cooper on the effect of bound electrons on the ground state of a fermionic sea. To study BCS theory, we need to first discuss about non-interacting fermi sea and Cooper problem.

i. The Non-Interacting Electron Gas

For any solid state system, the complete Hamiltonian is given by :

$$\begin{aligned} H &= H_{e-e} + H_{ion-ion} + H_{e-ion} \\ H_{e-e} &\rightarrow \text{ Hamiltonian for electrons moving through the solid} \\ H_{ion-ion} &\rightarrow \text{ Hamiltonian for ions in the solid} \\ H_{e-ion} &\rightarrow \text{ Hamiltonian describing the coupling between the electrons and the ions} \end{aligned}$$

Let m_e be electron mass and M be mass of ions :

$$\begin{aligned} H_{e-e} &= \sum_i \frac{p_i^2}{2m} + \sum_{i,j} V_{\text{Coulomb}}^{e-e}(\boldsymbol{r}_i - \boldsymbol{r}_j) \\ H_{ion-ion} &= \sum_i \frac{p_i^2}{2M} + \sum_{i,j} V_{\text{Coulomb}}^{ion-ion}(\boldsymbol{R}_i - \boldsymbol{R}_j) \\ H_{e-ion} &= V_{\text{Coulomb}}^{e-ion}(\boldsymbol{r}_i - \boldsymbol{R}_j) \end{aligned}$$

The dominant effect of $H_{ion-ion}$ is to fix the ions into a lattice. Once the ions are fixed, this Hamiltonian need not be considered.

We would describe the system using second quantisation. The fermionic creation $c_{\boldsymbol{k},\sigma}^\dagger$ and annihilation $c_{\boldsymbol{k},\sigma}$ for electrons with linear momentum $\boldsymbol{k}$ and spin σ are the basic building blocks.
$c_{\boldsymbol{k},\sigma}^\dagger$ creates a Bloch state and spin state with quantum number $(\boldsymbol{k}, \sigma)$; $c_{\boldsymbol{k},\sigma}$ annihilates the same. Also we know from before :

$$c_{\boldsymbol{k},\sigma}^\dagger c_{\boldsymbol{k'},\sigma'}^\dagger + c_{\boldsymbol{k'},\sigma'} c_{\boldsymbol{k},\sigma}^\dagger = \delta_{\boldsymbol{k},\boldsymbol{k'}} \delta_{\sigma,\sigma'}$$

$$\hat{n}_{\boldsymbol{k},\sigma} = c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma}$$

The energy of any state $(\boldsymbol{k}, \sigma)$ is given by $\varepsilon_{\boldsymbol{k},\sigma}$. The Hamiltonian of a non-interacting electron system of state $(\boldsymbol{k}, \sigma)$ is given by :

$$H = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k},\sigma} c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma}$$

If we assume the energy of the state to be independent of σ, i.e., $\varepsilon_{\boldsymbol{k},\sigma} = \varepsilon_{\boldsymbol{k}}$. Then :

$$H = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma}$$

Let the uppermost filled state state have energy $\varepsilon_{\boldsymbol{k}}$ and momentum $\boldsymbol{k_F}$. Let $|\phi_0\rangle$ be the ground state.

$$n_{\boldsymbol{k},\sigma}|\psi_0\rangle = \Theta(\varepsilon_F - \varepsilon_{\boldsymbol{k}})$$

Θ is the Heaviside step function :

$$\Theta(\varepsilon_F - \varepsilon_{\boldsymbol{k}}) = \begin{cases} 1 & \text{if } \varepsilon_F > \varepsilon_{\boldsymbol{k}} \\ 0 & \text{if } \varepsilon_F < \varepsilon_{\boldsymbol{k}} \end{cases}$$

If ε_F is the energy of the Fermi level, then this means that in ground state all levels below the Fermi level are occupied and all levels above the Fermi level are unoccupied.

ii. Cooper Problem

It is an artificial problem first considered by Leon Cooper.
Let us assume we have a non-interacting Fermi sea. Now we add two electrons with wave vectors $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ each electron with energy just above ε_F. They cannot have energy lower than that as we know from the past subsection, all energy levels $\varepsilon < \varepsilon_F$ will be filled at $T = 0$. The electrons do not interact with the Fermi sea but they interact amongst themselves. They attract each other if they are both within a small energy w_0 from the Fermi surface. They show no other interaction.

Say the first electron gives off phonon with wave vector $\vec{q}$. It represents the loss of momentum due to the interaction of the electron with the lattice.

$$\boldsymbol{k}_1 = \boldsymbol{k}_1' + \vec{q}\,; \qquad \boldsymbol{k}_1' \rightarrow \text{ new wave vector}$$

This phonon is absorbed by the second electron :

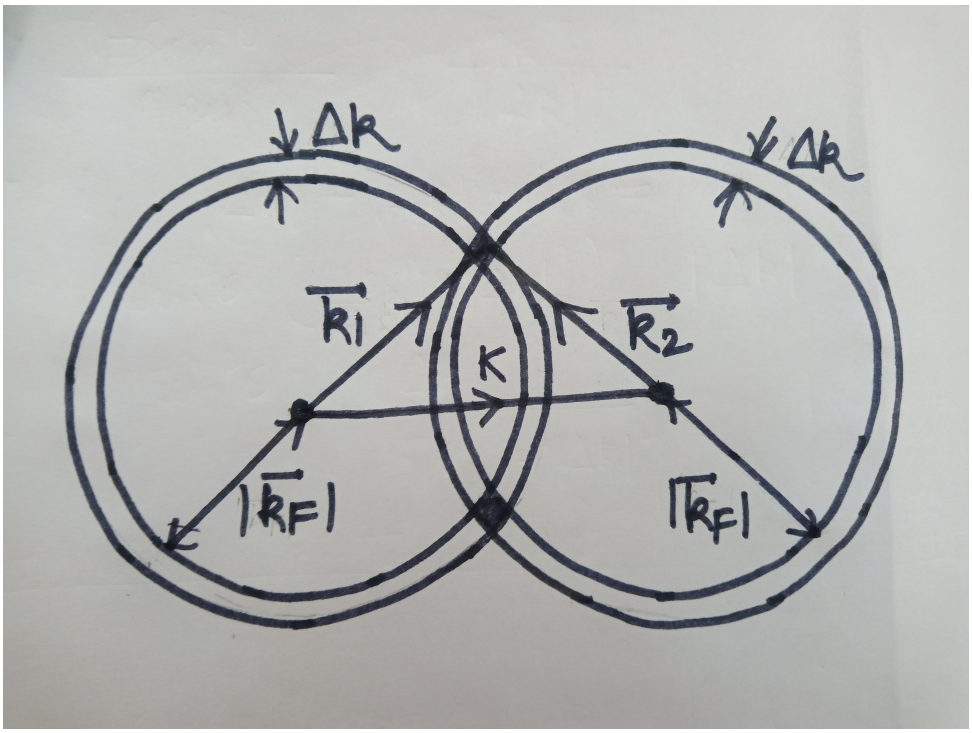
$$\boldsymbol{k}_2 + \vec{q} = \boldsymbol{k}_2'\,; \qquad \boldsymbol{k}_2' \rightarrow \text{ new wave vector}$$

This causes an effective attraction between the two electrons, with the momentum conserved.

$$\boldsymbol{k}_1 + \boldsymbol{k}_2 = \boldsymbol{k}_1' + \boldsymbol{k}_2' \equiv K$$

Let $\Delta\boldsymbol{k}$ be the maximum allowed momentum, i.e., $\vec{q} \leq \Delta\boldsymbol{k}$. Also, as all states below energy ε_F (consequently momentum $\boldsymbol{k}_F$) are filled, the new momentum of the electrons must follow :

$$\boldsymbol{k}_F \leq |\boldsymbol{k}_1'|, |\boldsymbol{k}_2'| \leq \boldsymbol{k}_F + \Delta\boldsymbol{k}$$
$$\boldsymbol{k}_F \leq |\boldsymbol{k}_1|, |\boldsymbol{k}_2| \leq \boldsymbol{k}_F + \Delta\boldsymbol{k}$$



Diagrammatic Representation of scattering from $\vec{k}_1$ and $\vec{k}_2$ in momentum space.

As K becomes smaller, the spherical shells overlap more. When K=0, then they completely overlap and the two electrons lie on opposite sides of the Fermi surface. So, $\boldsymbol{k}_1 = -\boldsymbol{k}_2 = \boldsymbol{k}$ (let).
So now we can consider the two electrons in Bloch states $|\boldsymbol{k}\rangle$ and $|-\boldsymbol{k}\rangle$ with energies greater than ε_F. They interact if they both lie within a small energy w_0 from the Fermi surface.

$$\text{max. } w_0 = \text{max. allowed energy of } \vec{q} \approx \hbar\omega_D$$

Otherwise they do not interact.
Hamiltonian of the system is given by :

$$H = H_0 + V_{eff}$$

If there is no interaction, then the Hamiltonian acts on the $|\boldsymbol{k}, -\boldsymbol{k}\rangle$:

$$H_0|\boldsymbol{k}, -\boldsymbol{k}\rangle = 2\varepsilon_{\boldsymbol{k}}|\boldsymbol{k}, -\boldsymbol{k}\rangle$$

$\varepsilon_{\boldsymbol{k}}$ is the single particle excitation energy of the non-interacting fermion system. $2\varepsilon_{\boldsymbol{k}} > 2\varepsilon_F$, as all lower states are filled.
In presence of interactions let the state be denoted by $|1, 2\rangle$. The Hamiltonian acting on this state :

$$H|1, 2\rangle = E|1, 2\rangle$$

E is the exact energy of the two particle state.
If $|\boldsymbol{k}, -\boldsymbol{k}\rangle$ form a complete basis, then the exact two particle eigen state $|1.2\rangle$ can be expanded in terms of this basis such that :

$$|1, 2\rangle = \sum_{\boldsymbol{k}} a_{\boldsymbol{k}}|\boldsymbol{k}, -\boldsymbol{k}\rangle$$

If we put this equation in the above Hamiltonian :

$$\begin{aligned}
H\left[\sum_{\boldsymbol{k}} a_{\boldsymbol{k}}|\boldsymbol{k}, -\boldsymbol{k}\rangle\right] &= E\left[\sum_{\boldsymbol{k}} a_{\boldsymbol{k}}|\boldsymbol{k}, -\boldsymbol{k}\rangle\right] \\
\implies (H_0 + V_{eff})\sum_{\boldsymbol{k}} a_{\boldsymbol{k}}|\boldsymbol{k}, -\boldsymbol{k}\rangle &= E\sum_{\boldsymbol{k}} a_{\boldsymbol{k}}|\boldsymbol{k}, -\boldsymbol{k}\rangle \\
\implies \sum_{\boldsymbol{k}} a_{\boldsymbol{k}} 2\varepsilon_{\boldsymbol{k}}|\boldsymbol{k}, -\boldsymbol{k}\rangle + \sum_{\boldsymbol{k}} a_{\boldsymbol{k}} V_{eff}|\boldsymbol{k}, -\boldsymbol{k}\rangle &= E\sum_{\boldsymbol{k}} a_{\boldsymbol{k}}|\boldsymbol{k}, -\boldsymbol{k}\rangle
\end{aligned}$$

Now we know that :

$$|\boldsymbol{k}, -\boldsymbol{k}\rangle = |\boldsymbol{k}\rangle \otimes |-\boldsymbol{k}\rangle$$

So, projecting this onto $\langle \boldsymbol{k'}, -\boldsymbol{k'}|$:

$$\begin{aligned}
\langle \boldsymbol{k'}, -\boldsymbol{k'}|\boldsymbol{k}, -\boldsymbol{k}\rangle &= (\langle \boldsymbol{k'}| \otimes \langle -\boldsymbol{k'}|)\,(|\boldsymbol{k}\rangle \otimes |-\boldsymbol{k}\rangle) \\
&= (\langle \boldsymbol{k'}|\boldsymbol{k}\rangle) \otimes (\langle -\boldsymbol{k'}|-\boldsymbol{k}\rangle) \\
\therefore \langle \boldsymbol{k'}, -\boldsymbol{k'}|\boldsymbol{k}, -\boldsymbol{k}\rangle &= \delta_{\boldsymbol{k},\boldsymbol{k'}}
\end{aligned}$$

So, projecting the Hamiltonian equation on $\langle \boldsymbol{k'}, -\boldsymbol{k'}|$:

$$\begin{aligned}
\sum_{\boldsymbol{k}} 2\varepsilon_{\boldsymbol{k}} a_{\boldsymbol{k}}\langle \boldsymbol{k'}, -\boldsymbol{k'}|\boldsymbol{k}, -\boldsymbol{k}\rangle + \sum_{\boldsymbol{k}} a_{\boldsymbol{k}}\langle \boldsymbol{k'}, -\boldsymbol{k'}|V_{eff}|\boldsymbol{k}, -\boldsymbol{k}\rangle &= E\sum_{\boldsymbol{k}} a_{\boldsymbol{k}}\langle \boldsymbol{k'}, -\boldsymbol{k'}|\boldsymbol{k}, -\boldsymbol{k}\rangle \\
\implies \sum_{\boldsymbol{k}} 2\varepsilon_{\boldsymbol{k}} a_{\boldsymbol{k}}\delta_{\boldsymbol{k},\boldsymbol{k'}} + \sum_{\boldsymbol{k}} a_{\boldsymbol{k}}\langle \boldsymbol{k'}, -\boldsymbol{k'}|V_{eff}|\boldsymbol{k}, -\boldsymbol{k}\rangle &= E\sum_{\boldsymbol{k}} a_{\boldsymbol{k}}\delta_{\boldsymbol{k},\boldsymbol{k'}} \\
\implies 2\varepsilon_{\boldsymbol{k'}} a_{\boldsymbol{k'}} - E a_{\boldsymbol{k'}} &= -\sum_{\boldsymbol{k}} a_{\boldsymbol{k}}\langle \boldsymbol{k'}, -\boldsymbol{k}|V_{eff}|_k, -\boldsymbol{k}\rangle
\end{aligned}$$

As $\boldsymbol{k}, \boldsymbol{k'}$ are dummy variables, we can write :

$$2\varepsilon_{\boldsymbol{k}} a_{\boldsymbol{k}} - E a_{\boldsymbol{k}} = -\sum_{k'} a_{\boldsymbol{k'}} \langle \boldsymbol{k}, -\boldsymbol{k} | V_{eff} | \boldsymbol{k'}, -\boldsymbol{k'} \rangle$$
$$a_{\boldsymbol{k}} \left[2\epsilon_{\boldsymbol{k}} - E \right] = -\sum_{\boldsymbol{k'}} a_{\boldsymbol{k'}} \langle \boldsymbol{k}, -\boldsymbol{k} | V_{eff} | \boldsymbol{k'}, -\boldsymbol{k'} \rangle$$

$\langle \boldsymbol{k}, -\boldsymbol{k} | V_{eff} | \boldsymbol{k'}, -\boldsymbol{k'} \rangle$ is a two particle scattering matrix. The two particles get scattered from state $|\boldsymbol{k'}, -\boldsymbol{k'}\rangle$ to $|\boldsymbol{k}, -\boldsymbol{k}\rangle$. We know that in our physical system, the two electrons have attractive interactions if they lie within a small energy from the surface, and have zero interaction everywhere else, so :

$$\langle \boldsymbol{k}, -\boldsymbol{k} | V_{eff} | \boldsymbol{k'}, -\boldsymbol{k'} \rangle = \begin{cases} -V & |\varepsilon_{\boldsymbol{k}} - \varepsilon_F| < \hbar\omega_D \quad \text{(V is positive)} \\ 0 & \text{otherwise} \end{cases}$$

Then we can write the above equation as :

$$a_{\boldsymbol{k}} \left[2\varepsilon_{\boldsymbol{k}} - E \right] = V \sum_{\boldsymbol{k'}} a_{\boldsymbol{k'}} \Theta \left(\varepsilon_{\boldsymbol{k}} - \varepsilon_F \right) \Theta \left(\hbar\omega_D - |\varepsilon_{\boldsymbol{k}} - \varepsilon_F| \right)$$

$\Theta(\varepsilon_{\boldsymbol{k}} - \varepsilon_F)$ ensures that $\varepsilon_{\boldsymbol{k}} > \varepsilon_F$, i.e., electron energy greater than Fermi surface energy.
$\Theta(\hbar\omega_D - |\varepsilon_{\boldsymbol{k}} - \varepsilon_F|)$ ensures that $\hbar > |\varepsilon_{\boldsymbol{k}} - \varepsilon_F|$, i.e., interaction operates in only a thin shell around the Fermi surface.
Let $N(\varepsilon)d\varepsilon$ be the weight factor such that we can transition from :

$$\sum_{\boldsymbol{k'}} \to \int_{-\infty}^{\infty} N(\varepsilon) d\varepsilon \; ; \quad \varepsilon_{\boldsymbol{k'}} \to \varepsilon \; ; \quad a_{\boldsymbol{k}} \to a$$

So now we can write :

$$a(\varepsilon) \left[2\varepsilon - E \right] = V \int_{-\infty}^{\infty} a(\varepsilon) N(\varepsilon) \Theta(\varepsilon - \varepsilon_F) \Theta(\hbar\omega_D - |\varepsilon - \varepsilon_F|) d\varepsilon$$

We can remove the Heaviside Step function from the equation if we set the limits appropriately, i.e., $\varepsilon > \varepsilon_F$ and $\varepsilon < \varepsilon_F + \hbar\omega_D$. Putting the limits accordingly we can write :

$$a(\varepsilon) \left[2\varepsilon - E \right] = V \int_{\varepsilon_F}^{\varepsilon_F + \hbar\omega_D} N(\varepsilon') a(\varepsilon') d\varepsilon'$$

Let us have an anstaz for $a(\varepsilon)$:

$$a(\varepsilon) = \frac{c}{2\varepsilon - E} \; ; \qquad c \to \text{ normalization constant}$$

If we replace $a(\varepsilon)$ by this anstaz :

$$1 = V \int_{\varepsilon_F}^{\varepsilon_F + \hbar\omega_D} \frac{N(\varepsilon')}{2\varepsilon' - E} d\varepsilon'$$

Let us now make the assumption that $N(\varepsilon)$ is constant in the energy range ε_F to $\varepsilon_F + \hbar\omega_D$. We also replace $N(\varepsilon)$ by $N(\varepsilon_F)$ and let λ be a dimensionless constant such that :

$$\lambda = VN(\varepsilon_F)$$

So, the above equation becomes :

$$\begin{aligned} 1 &= \lambda \int_{\varepsilon_F}^{\varepsilon_F + \hbar\omega_D} \frac{d\varepsilon'}{2\varepsilon' - E} \\ \implies 1 &= \lambda \ \ln\left[\frac{2(\varepsilon_F + \hbar\omega_D) - E}{2\varepsilon_F - E}\right] \end{aligned}$$

Let $2\varepsilon_F - E = \Delta$
It is the energy difference between energy of states of two non-interacting electrons at the Fermi surface and he exact energy of the interacting state of the two electrons.

$$\therefore \ \frac{1}{\lambda} = \ln\left[1 + \frac{2\hbar\omega_D}{\Delta}\right]$$

We must note that λ is a positive number as V is positive in our notation. So, $\dfrac{2\hbar\omega_D}{\Delta}$ must be positive, as $ln(x)$ for $x < 1$ is negative.
We already know that $\hbar\omega_D$ is positive, so for $\dfrac{2\hbar\omega_D}{\Delta}$ to be positive Δ must be positive, i.e.,

$$\Delta > 0 \quad \implies 2\varepsilon_F - E > 0 \quad \implies E < 2\varepsilon_F$$

The bound state resides at an energy prohibited by Pauli's Principle. Thus, on adding two electrons, interacting attractively, does not matter now weak the interaction is, produces an exact two particle state with total energy lower than twice the Fermi energy.
So we can conclude that the Fermi state is collapsing such that energy states below ε_F are becoming accessible.
Solving for Δ :

$$\begin{aligned} \frac{1}{\lambda} &= \ln\left[1 + \frac{\hbar\omega_D}{\Delta}\right] \\ \implies 1 + \frac{2\hbar\omega_D}{\Delta} &= e^{1/\lambda} \\ \implies \frac{2\hbar\omega_D}{\Delta} &= e^{1/\lambda} - 1 \end{aligned}$$

$$\implies \Delta = \frac{2\hbar\omega_D}{e^{1/\lambda} - 1}$$

If the interaction is weak, then $V \to 0$, then $\lambda \lll 1$, then $1/\lambda \to \infty$, then $e^{1/\lambda} \ggg 1$.

$$\text{Thus,} \quad \Delta = 2\hbar\omega_D e^{1/\lambda}$$

So, we see that Δ has an essential singularity as $\lambda \to 0$, as $e^{-1/x}$ does not have a Taylor series expansion about $x = 0$. Thus, an arbitrary weak attraction is a singular perturbation to the Fermi sea and it destabilizes it.
Also. if the Fermi sea vanishes then,

$$N(\varepsilon) \to 0 \implies a_{\boldsymbol{k}}[2\varepsilon_{\boldsymbol{k}} - E] \to 0 \implies 2\varepsilon_{\boldsymbol{k}} - E \to 0 \implies \Delta \to 0$$

Thus, there is no two electron bound state or arbitrary weak attraction in vacuum.
The pairing is a quantum effect because if $\hbar \to 0$, then $\Delta \to 0$.
We can also conclude that the quantum fluid of such Cooper pair electrons is not protected from interactions like the Fermi liquids obeying Pauli's principle.
Thus we can say that there could be a Ground State qualitatively different from the Free Electron Gas.

iii. Derivation of the BCS Gap Equation

We start by writing the Hamiltonian for electrons, in opposite spin-states and states of opposite linear momentum, interacting attractively (effective attraction mediated by phonons):

$$H + \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k'},\sigma,\sigma'} c_{\boldsymbol{k}+q,\sigma} c^\dagger_{\boldsymbol{k'}-q,\sigma'} c_{\boldsymbol{k},\sigma} c_{\boldsymbol{k'},\sigma'}$$

If this Hamiltonian has to produce a Cooper pair, then $\boldsymbol{k'} = \boldsymbol{k}$. Also, for the electrons to pair up they have to come very close in space, so by Pauli's Principle it is possible that the two electrons will have opposite spins, $\sigma' = \sigma$.
Pauli's principle tells us that like spin electrons repel each other and opposite spin electrons can come arbitrarily close to each other for strictly non-interacting electrons.

So, the Hamiltonian gets reduced to : (Replacing σ with $\uparrow$ and $-\sigma$ with $\downarrow$)

$$H = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k'}} V_{\boldsymbol{k},\boldsymbol{k'}} c^\dagger_{\boldsymbol{k},\uparrow} c^\dagger_{-\boldsymbol{k},\downarrow} c_{-\boldsymbol{k'},\downarrow} c_{\boldsymbol{k'},\uparrow}$$

The above equation is called the reduced BCS Hamiltonian.

$V_{\boldsymbol{k},\boldsymbol{k'}}$ is an attractive two-particle scattering matrix which is operative when both $\boldsymbol{k}$ and $\boldsymbol{k'}$ are within a thin shell around the Fermi surface.

The source of electrical resistivity in a pure metal is electron-phonon scattering. The source of superconductivity is the electron-phonon coupling leading to electron-electron attraction. Thus, the source of both above phenomenon is electron-phonon processes.

For superconductors the energy gap is a region of suppressed density of states around the Fermi energy. The size of the energy gap indicates the energy gain for two electrons upon formation of a Cooper pair. The energy gap is absent in temperatures above the critical temperature T_c; and it starts to open at temperature T_c and grows further as the temperature is reduced below T_c.

The superconducting gap is found by minimizing the expression for the free energy as a function of the gap parameter.

We first define the creation and annihilation operators for Cooper pairs.

$$b_{\boldsymbol{k}} \equiv \langle c_{-\boldsymbol{k},\downarrow} c_{\boldsymbol{k},\uparrow} \rangle$$
$$b_{\boldsymbol{k}}^\dagger \equiv \langle c_{\boldsymbol{k},\uparrow}^\dagger c_{-\boldsymbol{k},\downarrow}^\dagger \rangle$$

From these expectation values, we can write :

$$c_{-\boldsymbol{k},\downarrow} c_{\boldsymbol{k},\uparrow} = b_{\boldsymbol{k}} + \delta_{b_{\boldsymbol{k}}} \; ; \quad \delta_{b_{\boldsymbol{k}}} = c_{-\boldsymbol{k},\downarrow} c_{\boldsymbol{k},\uparrow} - b_{\boldsymbol{k}}$$
$$c_{\boldsymbol{k},\uparrow}^\dagger c_{-\boldsymbol{k},\downarrow}^\dagger = b_{\boldsymbol{k}}^\dagger + \delta_{b_{\boldsymbol{k}}^\dagger} \; ; \quad \delta_{b_{\boldsymbol{k}}^\dagger} = c_{\boldsymbol{k},\uparrow} c_{-\boldsymbol{k},\downarrow} - b_{\boldsymbol{k}}^\dagger$$

We insert the above relations into the effective Hamiltonian and we ignore terms of order $\mathcal{O}(\delta b_{\boldsymbol{k}}^2)$:

$$\begin{aligned}
H &= \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c_{\boldsymbol{k},\sigma}^\dagger c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k'}} V_{\boldsymbol{k},\boldsymbol{k'}} c_{\boldsymbol{k},\uparrow}^\dagger c_{-\boldsymbol{k},\downarrow}^\dagger c_{\boldsymbol{k'},\downarrow} c_{\boldsymbol{k'},\uparrow} \\
&= \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c_{\boldsymbol{k},\sigma}^\dagger c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k'}} V_{\boldsymbol{k},\boldsymbol{k'}} \left(b_{\boldsymbol{k'}} + \delta_{b_{\boldsymbol{k'}}} \right) \left(b_{\boldsymbol{k}}^\dagger + \delta_{b_{\boldsymbol{k}}^\dagger} \right) \\
&= \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c_{\boldsymbol{k},\sigma}^\dagger c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k'}} V_{\boldsymbol{k},\boldsymbol{k'}} \left(b_{\boldsymbol{k'}} b_{\boldsymbol{k}}^\dagger + b_{\boldsymbol{k'}} \delta_{b_{\boldsymbol{k}}^\dagger} + \delta_{b_{\boldsymbol{k'}}} b_{\boldsymbol{k}}^\dagger + \delta_{b_{\boldsymbol{k'}}} \delta_{b_{\boldsymbol{k}}^\dagger} \right) \\
&= \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c_{\boldsymbol{k},\sigma}^\dagger c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k'}} V_{\boldsymbol{k},\boldsymbol{k'}} \left(\cancel{b_{\boldsymbol{k'}} b_{\boldsymbol{k}}^\dagger} + b_{\boldsymbol{k'}} c_{\boldsymbol{k},\uparrow}^\dagger c_{-\boldsymbol{k},\downarrow}^\dagger - \cancel{b_{\boldsymbol{k'}} b_{\boldsymbol{k}}^\dagger} + b_{\boldsymbol{k}}^\dagger c_{-\boldsymbol{k},\downarrow} c_{\boldsymbol{k},\uparrow} - b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k'}} \right) \\
\therefore H &= \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c_{\boldsymbol{k},\sigma}^\dagger c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k'}} V_{\boldsymbol{k},\boldsymbol{k'}} \left(b_{\boldsymbol{k'}} c_{\boldsymbol{k},\uparrow}^\dagger c_{-\boldsymbol{k},\downarrow}^\dagger + b_{\boldsymbol{k}}^\dagger c_{-\boldsymbol{k},\downarrow} c_{\boldsymbol{k},\uparrow} - b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k'}} \right)
\end{aligned}$$

We introduce the superconductivity gap parameter, as follows :

$$\Delta_{\boldsymbol{k}}^\dagger \equiv - \sum_{\boldsymbol{k'}} V_{\boldsymbol{k},\boldsymbol{k'}} b_{\boldsymbol{k'}}^\dagger$$

$$\Delta_{\boldsymbol{k}} \equiv -\sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'} b_{\boldsymbol{k}'}$$

So, the Hamiltonian now becomes :

$$H = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} - \sum_{\boldsymbol{k}} \left(\Delta_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\uparrow} c^{\dagger}_{-\boldsymbol{k},\downarrow} + \Delta^{\dagger}_{\boldsymbol{k}} c_{-\boldsymbol{k},\downarrow} c_{\boldsymbol{k},\uparrow} - b^{\dagger}_{\boldsymbol{k}} \Delta_{\boldsymbol{k}} \right)$$

This is not yet in standard diagonal form of an effective non-interacting electron gas, so we perform a rotation of basis to diagonalise the Hamiltonian. We introduce two new fermion annihilation operators $(\eta_{\boldsymbol{k}}, \gamma_{\boldsymbol{k}})$:

$$\begin{aligned} c_{\boldsymbol{k},\uparrow} &= \cos(\theta)\eta_{\boldsymbol{k}} - \sin(\theta)\gamma_{\boldsymbol{k}} \\ c^{\dagger}_{\boldsymbol{k},\downarrow} &= \sin(\theta)\eta_{\boldsymbol{k}} + \cos(\theta)\gamma_{\boldsymbol{k}} \end{aligned}$$

Their corresponding adjoint operators are :

$$\begin{aligned} c^{\dagger}_{\boldsymbol{k},\downarrow} &= \cos(\theta)\eta^{\dagger}_{\boldsymbol{k}} - \sin(\theta)\gamma^{\dagger}_{\boldsymbol{k}} \\ c_{-\boldsymbol{k},\downarrow} &= \sin(\theta)\eta^{\dagger}_{\boldsymbol{k}} + \cos(\theta)\gamma^{\dagger}_{\boldsymbol{k}} \end{aligned}$$

Inserting these into the Hamiltonian we get :

$$\begin{aligned} H = &\sum_{\boldsymbol{k}} [\varepsilon_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}} b^{\dagger}_{\boldsymbol{k}}] \\ &+ \sum_{\boldsymbol{k}} \left[(\varepsilon_{\boldsymbol{k}} \cos(2\theta) - \sin(\theta)\cos(\theta))(\Delta_{\boldsymbol{k}} + \Delta^{\dagger}_{\boldsymbol{k}}) \right] \eta^{\dagger}_{\boldsymbol{k}} \eta_{\boldsymbol{k}} \\ &- \sum_{\boldsymbol{k}} \left[(\varepsilon_{\boldsymbol{k}} \cos(2\theta) - \sin(\theta)\cos(\theta))(\Delta_{\boldsymbol{k}} + \Delta^{\dagger}_{\boldsymbol{k}}) \right] \gamma^{\dagger}_{\boldsymbol{k}} \gamma_{\boldsymbol{k}} \\ &- \sum_{\boldsymbol{k}} \left[\Delta_{\boldsymbol{k}} \cos^2(\theta) - \Delta^{\dagger}_{\boldsymbol{k}} \sin^2(\theta) - 2\varepsilon_{\boldsymbol{k}} \sin(\theta)\cos(\theta) \right] \eta^{\dagger}_{\boldsymbol{k}} \gamma_{\boldsymbol{k}} \\ &- \sum_{\boldsymbol{k}} \left[\Delta^{\dagger}_{\boldsymbol{k}} \cos^2(\theta) - \delta_{\boldsymbol{k}} \sin^2(\theta) - 2\varepsilon_{\boldsymbol{k}} \sin(\theta)\cos(\theta) \right] \gamma^{\dagger}_{\boldsymbol{k}} \eta_{\boldsymbol{k}} \end{aligned}$$

We need to choose θ such that the Hamiltonian gets diagonalised, i.e., terms corresponding to $\eta_{\boldsymbol{k}}\gamma^{\dagger}_{\boldsymbol{k}}$ and $\eta^{\dagger}_{\boldsymbol{k}}\gamma_{\boldsymbol{k}}$ vanish. We can achieve this by setting $\Delta_{\boldsymbol{k}} = \Delta^{\dagger}_{\boldsymbol{k}}$ and choosing θ such that :

$$\tan(2\theta) = -\frac{\Delta_{\boldsymbol{k}}}{\varepsilon_k}$$

For such θ, we have :

$$\begin{aligned} \sin^2(\theta) \equiv \nu^2_{\boldsymbol{k}} &= \frac{1}{2}\left[1 - \frac{\varepsilon_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right] \\ \cos^2(\theta) \equiv \mu^2_{\boldsymbol{k}} &= \frac{1}{2}\left[1 + \frac{\varepsilon_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right] \\ E_{\boldsymbol{k}} &\equiv \sqrt{\varepsilon^2_{\boldsymbol{k}} + |\Delta k|^2} \end{aligned}$$

$\nu_{\boldsymbol{k}}^2$ and $\mu_{\boldsymbol{k}}^2$ are called coherence factors.
Putting this in the Hamiltonian :

$$\therefore\ H = \sum_{\boldsymbol{k}} (\varepsilon_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}} b_{\boldsymbol{k}}^\dagger) + \underbrace{\sum_{\boldsymbol{k}} E_{\boldsymbol{k}} \left[\eta_{\boldsymbol{k}}^\dagger \eta_{\boldsymbol{k}} - \gamma_{\boldsymbol{k}}^\dagger \gamma_{\boldsymbol{k}}\right]}_{\text{Hamiltonian for spinless fermions}}$$

The species are spinless because they are the linear combination of electrons and holes with opposite spins. $c_{\boldsymbol{k},\uparrow}$ represents a hole and $c_{-\boldsymbol{k},\downarrow}$ represents an electron.

$$\begin{pmatrix} \eta_{\boldsymbol{k}} \\ \gamma_{\boldsymbol{k}} \end{pmatrix} = \begin{pmatrix} \mu_{\boldsymbol{k}} & \nu_{\boldsymbol{k}} \\ -\nu_{\boldsymbol{k}} & \mu_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} c_{\boldsymbol{k},\uparrow} \\ c_{-\boldsymbol{k},\downarrow} \end{pmatrix}$$

The order parameter $\Delta_{\boldsymbol{k}}$ is non-zero in superconducting phase. $E_{\boldsymbol{k}} = \Delta_{\boldsymbol{k}}$ when $\varepsilon_{\boldsymbol{k}} = 0$, i.e., $\Delta_{\boldsymbol{k}}$ is the minimum energy of the gap in the ordered state. $\Delta_{\boldsymbol{k}}$ is referred to a superconducting gap.

This has now the form of a free fermion gas, we can write down the grand canonical partition function :

$$\begin{aligned} Z_g &= e^{-\beta H_0} \prod_{\boldsymbol{k}} (1 + e^{-\beta E_{\boldsymbol{k}}})(1 + e^{\beta E_{\boldsymbol{k}}}) = e^{-\beta F} \\ H_0 &\equiv \sum_{\boldsymbol{k}} [\varepsilon_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}} b_{\boldsymbol{k}}^\dagger] \end{aligned}$$

We can say from this that the free energy F of the system is given by :

$$F = H_0 - \frac{1}{\beta} \sum_{\boldsymbol{k}} [\ln(1 + e^{-\beta E_{\boldsymbol{k}}}) + \ln(1 + e^{\beta E_{\boldsymbol{k}}})]$$

This has the form of a pure mean-field term. Atzero temperature ($\beta \to \infty$), the entropic contribution to the free energy vanishes :

$$\begin{aligned} F &= H_0 + \sum_{\boldsymbol{k}} [E_{\boldsymbol{k}} \Theta(-E_{\boldsymbol{k}}) + E_{\boldsymbol{k}} \Theta(E_{\boldsymbol{k}})] \\ &= H_0 + \sum_{\boldsymbol{k}} [E_{bmk}(1 - \Theta(E_{\boldsymbol{k}})) - E_{\boldsymbol{k}} \Theta(E_{\boldsymbol{k}})] \\ &= \sum_{\boldsymbol{k}} [\varepsilon_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}} b_{\boldsymbol{k}}^\dagger - E_{\boldsymbol{k}}] \end{aligned}$$

The gap $\Delta_{\boldsymbol{k}}$ is determined by minimising the free energy with respect to the variations in $\Delta_{\boldsymbol{k}}$. We demand these to be satisfied for superconducting gaps :

$$\frac{\partial F}{\partial \Delta_{\boldsymbol{k}}} = 0$$

$$\frac{\partial F}{\partial \Delta_{\boldsymbol{k}}^{\dagger}} = 0$$

Applying these we obtain :

$$b_{\boldsymbol{k}}^{\dagger} + \frac{\partial E_{\boldsymbol{k}}}{\partial \Delta_{\boldsymbol{k}}} \left(\frac{e^{-\beta E_{\boldsymbol{k}}}}{1 + e^{-\beta E_{\boldsymbol{k}}}} - \frac{e^{\beta E_{\boldsymbol{k}}}}{1 + e^{\beta E_{\boldsymbol{k}}}} \right) = 0$$

Equivalently we can write :

$$b_{\boldsymbol{k}}^{\dagger} = \Delta_{\boldsymbol{k}} \underbrace{\frac{\tanh(\beta E_{\boldsymbol{k}}/2)}{2E_{\boldsymbol{k}}}}_{\equiv \chi(\boldsymbol{k})}$$

$\chi(\boldsymbol{k})$ is interpreted as pair-susceptibility, i.e., the ability of the system to form Cooper pairs. Using this, we finally arrive at the ***BCS Gap Equation*** :

$$\boxed{\Delta_{\boldsymbol{k}} = -\sum_{\boldsymbol{k'}} V_{\boldsymbol{k},\boldsymbol{k'}} \Delta_{\boldsymbol{k'}} \frac{\tanh(\beta E_{\boldsymbol{k'}}/2)}{2E_{\boldsymbol{k'}}}} \tag{18}$$

It applies at the mean-field level to any superconductor, if we donot specify the origin of attraction. It is not limited to phonon-meadiated superconductivity.

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