

Second Quantization

Second Quantization / Canonical Quantization is a formalism in which the Quantum fields are thought of field operators in a manner similar to how the physical quantities of particles like position, momentum, energy, etc are thought of as operators in the First Quantization procedure.

First quantization is a procedure for converting equations of classical particles equations into quantum operator & wave function equations, Interpreting classical particles as waves.

Second quantization is a procedure for converting equations of classical fields or waves into quantized excitations which are interpreted as particles.

Quantum Harmonic Oscillator

Consider a Quantum oscillator whose hamiltonian operator is given by,

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

Now we wish to factorize the above term as follows:

Define operators $\hat{a}$ & $\hat{a}^+$ such that

$$\hat{x} = \frac{x_0}{\sqrt{2}} (\hat{a}^+ + \hat{a}), \quad \hat{p}_x = \frac{i\hbar}{\sqrt{2}x_0} (\hat{a}^+ - \hat{a})$$

$$\text{Since } [\hat{x}, \hat{p}_x] = i\hbar$$

$$\Rightarrow \frac{i\hbar}{2} [\hat{a}^+ + \hat{a}, \hat{a}^+ - \hat{a}] = i\hbar$$

$$\Rightarrow \frac{[\hat{a}, \hat{a}^+] + [\hat{a}, \hat{a}^+]}{2} = 1$$

$$\Rightarrow \underline{[\hat{a}, \hat{a}^+] = 1} \Rightarrow \hat{a}\hat{a}^+ = \hat{a}^+\hat{a} + 1$$

And $\hat{H}$ is then given by,

$$\hat{H} = \hbar\omega \left[\hat{a}^\dagger \hat{a} + \frac{1}{2} \right]$$

$$\text{Let } \hat{N} = \hat{a}^\dagger \hat{a}, \quad \hat{N}^\dagger = \hat{N}$$

$$[\hat{N}, \hat{a}] = [\hat{a}^\dagger \hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}] \hat{a} = -\hat{a}$$

$$\rightarrow \underline{\hat{N} \hat{a} = \hat{a} (\hat{N} - \hat{I})}$$

$$\text{Similarly } [\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger$$

$$\& \underline{\hat{N} \hat{a}^\dagger = \hat{a}^\dagger (\hat{N} + \hat{I})}$$

$$\& \hat{H} = \hbar\omega \left[\hat{N} + \frac{1}{2} \right]$$

$$\Rightarrow [\hat{H}, \hat{N}] = 0$$

So $\hat{H}$ & $\hat{N}$ can be diagonalized together.

Let the eigen states of $\hat{N}$ be $\{|n\rangle\}$ with eigen value 'n'.

$$\Rightarrow \hat{N}|n\rangle = n|n\rangle$$

$$\begin{aligned}\text{Then, } \hat{N}(\hat{a}|n\rangle) &= \hat{a}(\hat{N} - \hat{I})|n\rangle \\ &= \hat{a}(n-1)|n\rangle\end{aligned}$$

$$\Rightarrow \underline{\hat{N}(\hat{a}|n\rangle) = (n-1)(\hat{a}|n\rangle)}$$

Thus $\hat{a}|n\rangle$ is also an eigenstate of $\hat{N}$ with eigen value 'n-1'.

$$\Rightarrow \underline{\hat{a}|n\rangle = C_-(n)|n-1\rangle}$$

$C_-(n)$ is some proportionality constant.

$$\begin{aligned}\text{Similarly, } \hat{N}(\hat{a}^+|n\rangle) &= \hat{a}^+(\hat{N} + \hat{I})|n\rangle \\ &= \hat{a}^+(n+1)|n\rangle\end{aligned}$$

$$\Rightarrow \hat{N}(\hat{a}^+|n\rangle) = (n+1)(\hat{a}^+|n\rangle)$$

$$\Rightarrow \underline{\hat{a}^+|n\rangle = C_+(n)|n+1\rangle}$$

Now, $\{|n\rangle\}$ forms an orthonormal basis. So, $\langle n|n'\rangle = \delta_{nn'}$

Thus we can find $C_-(n)$ & $C_+(n)$ as follows.

$$\hat{a}|n\rangle = C_-(n)|n-1\rangle$$

$$\Rightarrow \langle n|\hat{a}^\dagger = [C_-(n)]^* \langle n-1|$$

$$\Rightarrow \underbrace{\langle n|\hat{a}^\dagger \hat{a}|n\rangle}_{\hat{N}} = |C_-(n)|^2 \underbrace{\langle n-1|n-1\rangle}_1$$

$$\Rightarrow |C_-(n)|^2 = n$$

$\Rightarrow$ 'n' is always a +ve number.

$$\Rightarrow \underline{C_-(n) = e^{i\epsilon_g^{(-)}} \sqrt{n}}$$

$\epsilon_g^{(-)} \rightarrow$ some arbitrary phase.

$$\Rightarrow \hat{a}|n\rangle = e^{i\epsilon_g^{(-)}} \sqrt{n} |n-1\rangle$$

Similarly,

$$\hat{a}^+ |n\rangle = c_+(n) |n+1\rangle$$

$$\Rightarrow \langle n | \hat{a} = [c_+(n)]^* \langle n+1|$$

$$\Rightarrow \langle n | \underbrace{\hat{a} \hat{a}^+}_{\hat{N}+1} |n\rangle = |c_+(n)|^2 \underbrace{\langle n+1 | n+1 \rangle}_1$$

$$\Rightarrow |c_+(n)|^2 = n+1$$

$$\Rightarrow \underline{c_+(n) = e^{i\varepsilon_s^{(+)}} \sqrt{n+1}}$$

$\varepsilon_s \rightarrow$ some arbitrary phase.

$$\Rightarrow \hat{a}^+ |n\rangle = e^{i\varepsilon_s^{(+)}} \sqrt{n+1} |n+1\rangle$$

Consider $\hat{a}^+ \hat{a} |n\rangle = \hat{a}^+ e^{i\varepsilon_s^{(-)}} \sqrt{n} |n-1\rangle$

$$= e^{i\varepsilon_s^{(-)}} \sqrt{n} \hat{a}^+ |n-1\rangle$$
$$= e^{i\varepsilon_s^{(-)}} \sqrt{n} e^{i\varepsilon_s^{(+)}} \sqrt{n} |n\rangle$$

$$\Rightarrow \hat{a}^+ \hat{a} |n\rangle = e^{i[\varepsilon_s^{(-)} + \varepsilon_s^{(+)}]} n |n\rangle$$

$$\text{But } \hat{a}^\dagger \hat{a} |n\rangle = \hat{N} |n\rangle = n |n\rangle$$

Hermitian $\Rightarrow$ eigen value is real.

$$\text{Thus, } \mathcal{E}_g^{(-)} + \mathcal{E}_g^{(+)} = 0 \text{ is must.}$$

$$\text{Let } \mathcal{E}_g^{(+)} = -\mathcal{E}_g^{(-)} = \mathcal{E}_g.$$

$$\Rightarrow \hat{a}^\dagger |n\rangle = e^{i\mathcal{E}_g} \sqrt{n+1} |n+1\rangle$$

$$\& \hat{a} |n\rangle = e^{-i\mathcal{E}_g} \sqrt{n} |n-1\rangle$$

Acting ' $\hat{a}$ ' on $|n\rangle$ multiple times cannot lead to a -ve ' n '. The lowest value of ' n ' that can be achieved is $n=0$.

$\Rightarrow \hat{a} |0\rangle = 0 |0\rangle$, which prevents reaching -ve ' n ' values.

Thus choosing $|0\rangle$ as ground state is the only correct option.

Since we can have arbitrary, over all phase for a state, we can choose $|0\rangle$ such that ' $\mathcal{E}_g = 0$ '.

Thus we can write any state as,

$$\underline{|n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}} |0\rangle}$$

Thus we can summarize the results:

$$\hat{N}|n\rangle = n|n\rangle, \quad n = 0, 1, 2, 3, \dots$$

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$$

$$\hat{a}^+|n\rangle = \sqrt{n+1}|n+1\rangle$$

$$\hat{H}|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle$$

$$\Rightarrow E_n = \hbar\omega\left(n + \frac{1}{2}\right) \quad [n = 0, 1, 2, 3, \dots]$$

(Energy eigen values)

$$\{E_n\} = \left\{ \underbrace{\frac{\hbar\omega}{2}}_{\text{Ground state}}, \underbrace{\frac{3\hbar\omega}{2}, \frac{5\hbar\omega}{2}, \dots}_{\text{excited states}} \right\}$$

$$E_{n+1} - E_n = \hbar\omega \Rightarrow \text{Energy quantum}$$

We can call $\hat{a}^+$ as a creation operator which increases the energy of oscillator by one quanta $= \hbar\omega$.

$$\hat{H}(\hat{a}^+|n\rangle) = [E_n + \hbar\omega](\hat{a}^+|n\rangle)$$

Similarly $\hat{a}$ is called as Annihilation operator which decreases the energy of oscillator by one quanta $= \hbar\omega$.

$$\hat{H}(\hat{a}|n\rangle) = [E_n - \hbar\omega](\hat{a}|n\rangle)$$

These quanta behaves as particles with quantized energy of $\hbar\omega$.

And $\hat{N}$ tells how many quantum of energy is present in the oscillator. Hence, it is called number operator.

These quanta can be interpreted as particles; we can add / subtract them by the application of $\hat{a}$ & $\hat{a}^+$.

Many Non-Interacting quantum oscillators

Consider a set of 'M' number of coupled oscillators which are not interacting. So the only observable physical quantity is the energy of any oscillator and also the net Energy of all oscillators combined.

Let $\hat{H}_j$ be the hamiltonian of the j -th oscillator whose energy eigen states are given by $\{|n_j\rangle\}$ which live a j -th Hilbert Space.

If we consider the direct product of all the oscillator Subspace, then,

$$\begin{aligned} \text{Total Hamiltonian is } \hat{H} &= \sum_{j=1}^M \hat{H}_j \\ &= [\hat{H}_1 \otimes \hat{I}_2 \otimes \hat{I}_3 \dots \otimes \hat{I}_M] + [\hat{I}_1 \otimes \hat{H}_2 \otimes \hat{I}_3 \dots \otimes \hat{I}_M] + \\ &\quad \dots + [\hat{I}_1 \otimes \hat{I}_2 \otimes \hat{I}_3 \dots \otimes \hat{H}_M] \end{aligned}$$

$$\text{Each } \hat{H}_j = \hbar \omega_j \left[\hat{a}_j^\dagger \hat{a}_j + \frac{1}{2} \right]$$

where $\hat{a}_j$'s satisfy the following:

$$[\hat{a}_j, \hat{a}_i] = [\hat{a}_j^\dagger, \hat{a}_i^\dagger] = 0$$

$$\& \quad \underline{[\hat{a}_j, \hat{a}_i^\dagger] = \delta_{ij}}$$

The eigen states of $\hat{H}$ are of the form, $|n_1, n_2, n_3, \dots, n_m\rangle$ which is a direct product of all $\{|n_j\rangle\}$ which lives in the direct product space of all the oscillator Hilbert Space which is called as the 'FOCK SPACE'.

$$\begin{aligned} \Rightarrow \hat{a}_j |n_1, n_2, \dots, n_j, \dots, n_m\rangle \\ = \sqrt{n_j} |n_1, n_2, \dots, n_j - 1, \dots, n_m\rangle \end{aligned}$$

$$\begin{aligned} \& \hat{a}_j^\dagger |n_1, n_2, \dots, n_j, \dots, n_m\rangle \\ = \sqrt{n_j + 1} |n_1, n_2, \dots, n_j + 1, \dots, n_m\rangle \end{aligned}$$

The state with all the oscillators in the ground state is given by the vacuum state denoted by

$$|\Omega\rangle = |0, 0, 0, \dots, 0\rangle$$

Then any general state $|n_1, n_2, \dots, n_M\rangle$ can be written as

$$|n_1, n_2, \dots, n_M\rangle = \frac{(\hat{a}_1^\dagger)^{n_1} (\hat{a}_2^\dagger)^{n_2} \dots (\hat{a}_M^\dagger)^{n_M} |\Omega\rangle}{\sqrt{n_1! n_2! \dots n_M!}}$$

Compactly we can express,

$$|\{n_i\}\rangle = \prod_{j=1}^M \frac{(\hat{a}_j^\dagger)^{n_j}}{\sqrt{n_j!}} |\Omega\rangle$$

We should make sure that, j^{th} oscillator contains n_j quanta by maintaining the order.

The total number operator is

$\hat{N} = \sum_j \hat{a}_j^\dagger \hat{a}_j$ which gives the total number of quanta in all the oscillators.

$$\Rightarrow \hat{N} |\{n_i\}\rangle = \left(\sum_j n_j \right) |\{n_i\}\rangle$$

Total energy operator is

$$\hat{H} = \sum_{j=1}^M \hbar \omega_j \left[\hat{N}_j + \frac{1}{2} \right]$$

where $\hat{N}_j = \hat{a}_j^\dagger \hat{a}_j$

$\hat{N}_j$ gives number of quanta in j^{th} oscillator.

Phonons

Consider a linear chain of 'N' atoms each of identical mass 'm'. They are all connected by identical springs of spring constant 'K' & length 'l'. So a j^{th} atom in its equilibrium state is located at a distance $R_j = jl$ from the origin, but can be displaced by a small amount x_j . The momentum of j^{th} atom is p_j .

The Hamiltonian for this system is,

$$\hat{H} = \sum_j \left[\frac{\hat{p}_j^2}{2m} + \frac{1}{2} K (x_{j+1} - x_j)^2 \right]$$

Thus we have a coupled oscillator system & we need to find its energy spectrum.

We begin by the discrete fourier transform of both $\hat{x}_j$ & $\hat{p}_j$

$\tilde{x}_k \Rightarrow$ fourier transformed operator of $\hat{x}_j$'s

$\tilde{p}_k \Rightarrow$ fourier transformed operator of $\hat{p}_j$'s

$$\tilde{x}_k = \frac{1}{\sqrt{N}} \sum_{m=1}^N \hat{x}_m e^{iklm}$$

$$\tilde{p}_k = \frac{1}{\sqrt{N}} \sum_{m=1}^N \hat{p}_m e^{iklm}$$

We shall impose periodic boundary condition, i.e., $e^{ika(m+N)} = e^{ikam}$

$$\Rightarrow e^{iklN} = 1$$

$$\Rightarrow kN = j\pi \quad (j \in \text{Integer})$$

$$k = \frac{j\pi}{N}, \quad -\frac{N}{2} < j < \frac{N}{2}$$

($N \rightarrow \text{even}$)

Then, the inverse fourier transform is given by,

$$\hat{x}_j = \frac{1}{\sqrt{N}} \sum_k \tilde{x}_k e^{ikR_j}$$

$$\hat{p}_j = \frac{1}{\sqrt{N}} \sum_k \tilde{p}_k e^{ikR_j}$$

$$\Rightarrow \frac{1}{N} \sum_{m=1}^N e^{i(k-k')lm} = \delta_{kk'}$$

$$\& \frac{1}{N} \sum_k e^{i(m-j)kl} = \delta_{mj}$$

The commutation relations are given by,

$$[\hat{x}_j, \hat{p}_m] = i\hbar \delta_{jm}$$

$$\Rightarrow [\tilde{x}_k, \tilde{p}_{k'}] = i\hbar \delta_{k, -k'}$$

$$\begin{aligned}
 \text{Since } [\tilde{x}_k, \tilde{p}_{k'}] &= \\
 &= \frac{1}{N} \sum_{j=1}^N \sum_{m=1}^N e^{il(kj+k'm)} \underbrace{[\hat{x}_j, \hat{p}_m]}_{i\hbar \delta_{jm}} \\
 &= \frac{i\hbar}{N} \sum_{m=1}^N e^{il(k+k')m} = i\hbar \delta_{k, -k'}
 \end{aligned}$$

$$\Rightarrow \underline{[\tilde{x}_k, \tilde{p}_{k'}] = i\hbar \delta_{k, -k'}}$$

Now we need to work out for the terms in hamiltonian,

$$\begin{aligned}
 \sum_j \hat{p}_j^2 &= \sum_j \frac{1}{N} \sum_{k, k'} \tilde{p}_k \tilde{p}_{k'} e^{i(k+k')lj} \\
 &= \sum_{k, k'} \tilde{p}_k \tilde{p}_{k'} \underbrace{\frac{1}{N} \sum_j e^{i(k+k')lj}}_{\delta_{k, -k'}}
 \end{aligned}$$

$$\Rightarrow \underline{\sum_j \hat{p}_j^2 = \sum_k \tilde{p}_k \tilde{p}_{-k}}$$

Similarly,

$$\sum_j (x_{j+1} - x_j) = \sum_j \sum_k \frac{\tilde{x}_k}{\sqrt{N}} (1 - e^{ikl}) e^{iklj}$$

$$\Rightarrow \sum_j (x_{j+1} - x_j)^2$$

$$= \sum_j \sum_{k, k'} \frac{\tilde{x}_k \tilde{x}_{k'}}{N} (1 - e^{ikl}) (1 - e^{ik'l}) e^{i(k+k')jl}$$

$$= \sum_{k, k'} \tilde{x}_k \tilde{x}_{k'} (1 - e^{ikl}) (1 - e^{ik'l}) \underbrace{\sum_j \frac{e^{i(k+k')jl}}{N}}_{\delta_{k, -k'}}$$

$$= \sum_k \tilde{x}_k \tilde{x}_{-k} \underbrace{(1 - e^{ikl}) (1 - e^{-ikl})}_{2[1 - \cos(kl)]}$$

$$\Rightarrow \sum_j (x_{j+1} - x_j)^2 = 2 \sum_k [1 - \cos(kl)] \tilde{x}_k \tilde{x}_{-k}$$

$$\hat{x}^+ = \hat{x} \Rightarrow \tilde{x}_{-k} = \tilde{x}_k^+$$

$$\hat{p}^+ = \hat{p} \Rightarrow \tilde{p}_{-k} = \tilde{p}_k^+$$

$$\Rightarrow \underbrace{[\tilde{x}_k, \tilde{p}_{k'}^+]} = i\hbar \delta_{k, k'}$$

Then, in terms of $\tilde{x}_k$'s & $\tilde{p}_k$'s

$$\hat{H} = \sum_j \left[\frac{\hat{p}_j^2}{2m} + \frac{1}{2} K (x_{j+1} - x_j)^2 \right]$$

can be written as,

$$\hat{H} = \sum_k \left[\frac{\tilde{p}_k \tilde{p}_k^+}{2m} + K [1 - \cos(kl)] \tilde{x}_k \tilde{x}_k^+ \right]$$

$$\text{Let } \underbrace{[\omega(k)]^2 = \frac{2K}{m} [1 - \cos(kl)]}$$

$$\Rightarrow \hat{H} = \sum_k \left[\frac{\tilde{p}_k \tilde{p}_k^+}{2m} + \frac{1}{2} m [\omega(k)]^2 \tilde{x}_k \tilde{x}_k^+ \right]$$

Then we can write the creation & annihilation operators as follows,

$$\tilde{x}_k = \frac{x_0(k)}{\sqrt{2}} (\hat{a}_k^+ + \hat{a}_k)$$

$$\& \quad \tilde{p}_k = \frac{i\hbar}{\chi_0(k)\sqrt{2}} (\hat{a}_k^+ - \hat{a}_k)$$

$$\text{where } \chi_0(k) = \sqrt{\frac{\hbar}{m\omega(k)}}$$

The commutation relations between $\hat{a}_k$'s & $\hat{a}_k^+$'s are:

$$\underline{[\hat{a}_k, \hat{a}_{k'}] = [\hat{a}_k^+, \hat{a}_{k'}^+] = 0}$$

$$\& \quad \underline{[\hat{a}_k, \hat{a}_{k'}^+] = \delta_{k,k'}}$$

Then,

$$\tilde{p}_k \tilde{p}_k^+ = \frac{i\hbar}{\chi_0(k)\sqrt{2}} (\hat{a}_k^+ - \hat{a}_k) \frac{(-i\hbar)}{\chi_0(k)\sqrt{2}} (\hat{a}_k - \hat{a}_k^+)$$

$$= \frac{\hbar^2}{2\chi_0(k)^2} [\hat{a}_k^+ \hat{a}_k - \hat{a}_k^2 - (\hat{a}_k^+)^2 + \hat{a}_k \hat{a}_k^+]$$

$$\Rightarrow \frac{\tilde{p}_k \tilde{p}_k^+}{2m} = \frac{\hbar\omega(k)}{4} [\hat{a}_k^+ \hat{a}_k + \hat{a}_k \hat{a}_k^+ - \hat{a}_k^2 - (\hat{a}_k^+)^2]$$

Similarly,

$$\begin{aligned}\tilde{x}_k \tilde{x}_k^+ &= \frac{[\chi_0(k)]^2}{2} (\hat{a}_k^+ + \hat{a}_k)^2 \\ &= \frac{[\chi_0(k)]^2}{2} \left[(\hat{a}_k^+)^2 + (\hat{a}_k)^2 + (\hat{a}_k^+ \hat{a}_k + \hat{a}_k \hat{a}_k^+) \right]\end{aligned}$$

$$\begin{aligned}\Rightarrow \frac{1}{2} m \omega(k)^2 \tilde{x}_k \tilde{x}_k^+ \\ = \frac{\hbar \omega(k)}{4} \left[(\hat{a}_k^+)^2 + (\hat{a}_k)^2 + (\hat{a}_k^+ \hat{a}_k + \hat{a}_k \hat{a}_k^+) \right]\end{aligned}$$

Then the Hamiltonian in terms of $\hat{a}_k$ & $\hat{a}_k^+$ is:

$$\hat{H} = \sum_k \frac{\hbar \omega(k)}{2} (\hat{a}_k^+ \hat{a}_k + \hat{a}_k \hat{a}_k^+)$$

But $\hat{a}_k \hat{a}_k^+ = 1 + \hat{a}_k^+ \hat{a}_k \}$ $\hat{N}_k \rightarrow$ Number operator

Thus the Hamiltonian reduces to

$$\hat{H} = \sum_k \hbar \omega(k) \left[\hat{a}_k^+ \hat{a}_k + \frac{1}{2} \right]$$

where $[\omega(k)]^2 = \frac{2K}{m} [1 - \cos(kl)]$

Thus the Hamiltonian for a 1D chain of atoms can be expressed in terms of sum over all possible modes ' k ' $\rightarrow$ wave vector.

These modes are called Phonons, & each phonon mode is labelled by a wave vector ' k ', & behave as a independent oscillator of frequency $\omega(k)$ & whose quanta of energy is $\hbar\omega(k)$ & phonon of mode ' k ' can have energy of $\frac{\hbar\omega(k)}{2} + \text{integer multiple of } \hbar\omega(k)$

Thus we can think of phonons as particles with quantized energy which behave as Bosonic particles. Hence problems of oscillators reduces to that of corresponding particles (quanta)

Change of Basis for ladder operators

Let $\{|\lambda_i\rangle\}$ and $\{|\rho_i\rangle\}$ be any two different orthonormal basis states of a single particle.

$$\Rightarrow \sum_i |\rho_i\rangle \langle \rho_i| = 1 \quad \& \quad \sum_i |\lambda_i\rangle \langle \lambda_i| = 1$$

They also have corresponding creation & annihilation operators as shown:

$\hat{a}_{\lambda_i}^+ \rightarrow$ creates a single particle in the quantum state ' λ_i '

$\hat{a}_{\lambda_i} \rightarrow$ annihilates a particle in the quantum state ' λ_i '

$$\Rightarrow |\lambda_i\rangle = \hat{a}_{\lambda_i}^+ |\Omega\rangle \quad \& \quad \langle \lambda_i| = \langle \Omega| \hat{a}_{\lambda_i}$$

Similarly, $\hat{a}_{\rho_i}^+ |\Omega\rangle = |\rho_i\rangle$
& $\langle \rho_i| = \langle \Omega| \hat{a}_{\rho_i}$

The relation b/w $\{|\lambda_i\rangle\}$ & $\{|\rho_i\rangle\}$ is unitary (related by unitary matrix)

$$\Rightarrow |\rho_i\rangle = \sum_j |\lambda_j\rangle \langle \lambda_j | \rho_i \rangle$$

$$\Rightarrow \hat{a}_{\rho_i}^+ |\Omega\rangle = \sum_j \langle \lambda_j | \rho_i \rangle \hat{a}_{\lambda_j}^+ |\Omega\rangle$$

$$\Rightarrow \boxed{\hat{a}_{\rho_i}^+ = \sum_j \langle \lambda_j | \rho_i \rangle \hat{a}_{\lambda_j}^+}$$

$$\& \boxed{\hat{a}_{\rho_i} = \sum_j \langle \rho_i | \lambda_j \rangle \hat{a}_{\lambda_j}}$$

The inverse relation is:

$$\boxed{\hat{a}_{\lambda_i}^+ = \sum_j \langle \rho_j | \lambda_i \rangle \hat{a}_{\rho_j}^+}$$

$$\& \boxed{\hat{a}_{\lambda_i} = \sum_j \langle \lambda_i | \rho_j \rangle \hat{a}_{\rho_j}}$$

Thus we can relate the creation & annihilation operators in various basis.

Second quantizing an operator

Consider a single particle operator $\hat{A}$ which is diagonal in some basis $\{|\lambda_i\rangle\}$ that are the quantum states of a single particle.

$$\rightarrow \hat{A} = \sum_i A_i |\lambda_i\rangle \langle \lambda_i|$$

where $\hat{A}|\lambda_i\rangle = A_i |\lambda_i\rangle$ & $\langle \lambda_i| \hat{A} |\lambda_i\rangle = A_i$

In second quantization language,

$\hat{a}_{\lambda_i}^+ \rightarrow$ creates a single particle in the quantum state ' λ_i '

$\hat{a}_{\lambda_i} \rightarrow$ annihilates a particle in the quantum state ' λ_i '

$$\Rightarrow |\lambda_i\rangle = \hat{a}_{\lambda_i}^+ |\Omega\rangle$$

$$\& \langle \lambda_i| = \langle \Omega| \hat{a}_{\lambda_i}$$

Let $|n_{\lambda_1}, n_{\lambda_2}, n_{\lambda_3}, \dots\rangle$ be the state of a many body system in Fock basis. where $\{\lambda_i\}$ are allowed states of a single particle.

$$\rightarrow \sum_{\{n_{\lambda_i}\}} |n_{\lambda_1}, n_{\lambda_2}, n_{\lambda_3}, \dots\rangle \langle n_{\lambda_1}, n_{\lambda_2}, n_{\lambda_3}, \dots| = 1$$

Now if we need the second quantized action of $\hat{A}$, then, we should find action of $\hat{A}$ on all particles & then sum over them.

$\hat{n}_{\lambda_i} \rightarrow$ gives number of particles in the state λ_i

Then, $\langle n_{\lambda_1}, n_{\lambda_2}, n_{\lambda_3}, \dots | \hat{A} | n_{\lambda_1}, n_{\lambda_2}, n_{\lambda_3}, \dots \rangle$ gives total expectation value of $\hat{A}$.

$$\rightarrow \hat{A} = \sum_i A_i \hat{n}_{\lambda_i}$$

(In 2nd quantized language)

But $\hat{n}_{\lambda_i} = \hat{a}_{\lambda_i}^\dagger \hat{a}_{\lambda_i}$ is the number operator which gives the number of particles in the state λ_i .

Thus in the diagonal basis of $\hat{A}$

$$\Rightarrow \hat{A} = \sum_i A_i \hat{a}_{\lambda_i}^\dagger \hat{a}_{\lambda_i}$$

Let $\{|P_i\rangle\}$ be an arbitrary O.N. basis which satisfies, $\sum_i |P_i\rangle \langle P_i| = 1$

They also have corresponding creation & annihilation operators $\hat{a}_{P_i}^\dagger$ and $\hat{a}_{P_i}$.

$$\Rightarrow \hat{a}_{P_i}^\dagger |\Omega\rangle = |P_i\rangle \quad \& \quad \langle P_i| = \langle \Omega| \hat{a}_{P_i}$$

The relation b/w $\{|\lambda_i\rangle\}$ & $\{|P_i\rangle\}$

is unitary $\Rightarrow |\lambda_i\rangle = \sum_j |P_j\rangle \langle P_j|\lambda_i\rangle$

Similarly, $\hat{a}_{\lambda_i}^+ = \sum_j \langle p_j | \lambda_i \rangle \hat{a}_{p_j}^+$

& $\hat{a}_{\lambda_i} = \sum_j \langle \lambda_i | p_j \rangle \hat{a}_{p_j}$

$$\Rightarrow \hat{A} = \sum_i A_i \hat{a}_{\lambda_i}^+ \hat{a}_{\lambda_i}$$

$$= \sum_i A_i \sum_j \langle p_j | \lambda_i \rangle \hat{a}_{p_j}^+ \sum_l \langle \lambda_i | p_l \rangle \hat{a}_{p_l}$$

$$= \sum_j \sum_l \hat{a}_{p_j}^+ \hat{a}_{p_l} \sum_i \langle p_j | \lambda_i \rangle A_i \langle \lambda_i | p_l \rangle$$

$$= \sum_{j,l} \hat{a}_{p_j}^+ \hat{a}_{p_l} \sum_i \langle p_j | \lambda_i \rangle \langle \lambda_i | \hat{A} | p_l \rangle$$

$$= \sum_{j,l} \hat{a}_{p_j}^+ \hat{a}_{p_l} \langle p_j | \hat{A} | p_l \rangle$$

$$\Rightarrow \boxed{\hat{A} = \sum_{j,l} A_{jl} \hat{a}_{p_j}^+ \hat{a}_{p_l}}$$

where $A_{jl} = \langle p_j | \hat{A} | p_l \rangle$

Thus $\hat{A}$ scatters $|p_l\rangle$ state to $|p_j\rangle$ with a probability amplitude ' A_{jl} '

Field Operators (Non-Relativistic limit)

We have seen in the previous case of non-relativistic oscillators that, we can convert many oscillator problem to a quantized particle problem by using the creation & annihilation operators.

$\hat{a}^+(\vec{p}) \rightarrow$ creates a particle with momentum $\vec{p}$

i.e. $\hat{a}^+(\vec{p})|\Omega\rangle$ is a state where a single particle of momentum ' $\vec{p}$ ' is present in the momentum space.
($|\Omega\rangle \Rightarrow$ Vacuum)

& $\hat{a}(\vec{p}) \rightarrow$ Annihilates a particle with momentum $\vec{p}$

Then by fourier transform of these operators we can obtain field operators denoted by $\hat{\psi}(\vec{x})$ & $\hat{\psi}^+(\vec{x})$.

$$\hat{\psi}(\vec{x}) = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\vec{p}} \hat{a}(\vec{p}) e^{i\vec{p} \cdot \vec{x}}$$

$$\& \hat{\psi}^+(\vec{x}) = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\vec{p}} \hat{a}^+(\vec{p}) e^{-i\vec{p} \cdot \vec{x}}$$

where ' $\mathcal{V}$ ' is some normalization constant such that:

$$\frac{1}{\mathcal{V}} \sum_{\vec{p}} e^{-i\vec{p} \cdot (\vec{x} - \vec{y})} = \delta(\vec{x} - \vec{y})$$

We can think of $\hat{\psi}^+(\vec{x})$ to create a particle at position ' $\vec{x}$ ' & $\hat{\psi}(\vec{x})$ to annihilate a particle present at ' $\vec{x}$ '.

If $|\vec{x}\rangle = \hat{\psi}^+(\vec{x})|\Omega\rangle$, then we get $\langle\vec{y}|\vec{x}\rangle = \delta(\vec{x} - \vec{y})$, which implies that $|\vec{x}\rangle$ corresponds to a single particle localized at $\vec{x}$.

$$\hat{\psi}^+(\vec{x})|\Omega\rangle = \frac{1}{\sqrt{V}} \sum_{\vec{p}} e^{-i\vec{p}\cdot\vec{x}} \hat{a}^+(\vec{p})|\Omega\rangle$$

$$\langle\Omega|\hat{\psi}(\vec{y}) = \frac{1}{\sqrt{V}} \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{y}} \langle\Omega|\hat{a}(\vec{q})$$

$$\Rightarrow \langle\vec{y}|\vec{x}\rangle = \langle\Omega|\hat{\psi}(\vec{y})\hat{\psi}^+(\vec{x})|\Omega\rangle$$

$$= \frac{1}{V} \sum_{\vec{p}, \vec{q}} e^{i(\vec{q}\cdot\vec{y} - \vec{p}\cdot\vec{x})} \langle\Omega|\hat{a}(\vec{q})\hat{a}^+(\vec{p})|\Omega\rangle$$

$\hat{a}^+(\vec{p})|\Omega\rangle \rightarrow$ single particle localized at $\vec{p}$ in momentum space.

$$\rightarrow \hat{a}^+(\vec{p})|\Omega\rangle = |\vec{p}\rangle \quad \& \quad \langle\Omega|\hat{a}(\vec{q}) = \langle\vec{q}|$$

$$\rightarrow \langle\Omega|\hat{a}(\vec{q})\hat{a}^+(\vec{p})|\Omega\rangle = \langle\vec{q}|\vec{p}\rangle = \delta(\vec{q} - \vec{p})$$

$$\begin{aligned} \rightarrow \langle\vec{y}|\vec{x}\rangle &= \frac{1}{V} \sum_{\vec{p}, \vec{q}} e^{i(\vec{q}\cdot\vec{y} - \vec{p}\cdot\vec{x})} \delta(\vec{q} - \vec{p}) \\ &= \frac{1}{V} \sum_{\vec{p}} e^{-i\vec{p}\cdot(\vec{x} - \vec{y})} = \delta(\vec{x} - \vec{y}) \end{aligned}$$

$$\Rightarrow \underline{\langle\vec{y}|\vec{x}\rangle = \delta(\vec{x} - \vec{y})}$$

Bosonic Field

$$\text{If } [\hat{a}(\vec{p}), \hat{a}(\vec{q})] = [\hat{a}^\dagger(\vec{p}), \hat{a}^\dagger(\vec{q})] = 0$$

$$\& [\hat{a}(\vec{p}), \hat{a}^\dagger(\vec{q})] = \delta(\vec{p} - \vec{q})$$

$$\rightarrow [\hat{\psi}(\vec{x}), \hat{\psi}(\vec{y})] = [\hat{\psi}^\dagger(\vec{x}), \hat{\psi}^\dagger(\vec{y})] = 0$$

$$\& [\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{y})] = \delta(\vec{x} - \vec{y})$$

Fermionic Field

$$\text{If } \{\hat{a}(\vec{p}), \hat{a}(\vec{q})\} = \{\hat{a}^\dagger(\vec{p}), \hat{a}^\dagger(\vec{q})\} = 0$$

$$\& \{\hat{a}(\vec{p}), \hat{a}^\dagger(\vec{q})\} = \delta(\vec{p} - \vec{q})$$

$$\rightarrow \{\hat{\psi}(\vec{x}), \hat{\psi}(\vec{y})\} = \{\hat{\psi}^\dagger(\vec{x}), \hat{\psi}^\dagger(\vec{y})\} = 0$$

$$\& \{\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{y})\} = \delta(\vec{x} - \vec{y})$$

where $\{$, $\}$ is anti-commutator