Creation & annihilation operators

It will be useful to define operators that add or remove particles from any given single particle state $|\alpha\rangle$.

For bosons for each such $|\alpha\rangle$, define operators with the algebra $[a_\alpha, a_\alpha^\dagger] = 1$ such that

$$a_\alpha |n_\alpha = 0\rangle = 0 .$$

i.e a_α annihilates the state if it is not occupied.

$$[a_\alpha, a_\alpha^\dagger] |n_\alpha = 0\rangle = |0_\alpha\rangle$$

$$\text{RHS} = a_\alpha a_\alpha^\dagger |0_\alpha\rangle$$

Let $a_\alpha^\dagger |0_\alpha\rangle = |1_\alpha\rangle$, $a_\alpha |1_\alpha\rangle = |0_\alpha\rangle$.

Compute $(a_\alpha^\dagger a_\alpha) |1_\alpha\rangle = a_\alpha^\dagger |0_\alpha\rangle = |1_\alpha\rangle$.

$\therefore$ $|1_\alpha\rangle$ is an eigenstate of $a_\alpha^\dagger a_\alpha$ with eigenvalue 1.

Note $|0_\alpha\rangle$ is an eigenstate of $a^\dagger_\alpha a_\alpha$ with eigenvalue 0.

Identify $\hat{n}_\alpha = a^\dagger_\alpha a_\alpha$; $\hat{n}_\alpha$ will have integer eigenvalues 0, 1, 2, ...

Proof: Let $\hat{n}_\alpha |n_\alpha\rangle = n_\alpha |n_\alpha\rangle$ where n_α = non-negative integer

$$\Rightarrow a^\dagger_\alpha a_\alpha |n_\alpha\rangle = n_\alpha |n_\alpha\rangle$$

$$\text{RHS} = \left(a_\alpha a^\dagger_\alpha - 1\right)|n_\alpha\rangle \Rightarrow a_\alpha a^\dagger_\alpha |n_\alpha\rangle = \left(1+n_\alpha\right)|n_\alpha\rangle$$

$$\Rightarrow \left(a^\dagger_\alpha a_\alpha\right)\left(a^\dagger_\alpha |n_\alpha\rangle\right) = \left(1+n_\alpha\right) a^\dagger_\alpha |n_\alpha\rangle.$$

$\therefore$ $a^\dagger_\alpha |n_\alpha\rangle$ is an eigenstate of $a^\dagger_\alpha a_\alpha = \hat{n}_\alpha$ with eigenvalue $\left(1+n_\alpha\right)$.

To normalize consider $\langle n_\alpha | a_\alpha a^\dagger_\alpha | n_\alpha\rangle = 1+n_\alpha$

(assuming $|n_\alpha\rangle$ is normalized).

$$\Rightarrow \quad |n_\alpha + 1\rangle = \frac{a_\alpha^\dagger |n_\alpha\rangle}{\sqrt{n_\alpha + 1}}$$

$$\Rightarrow \quad \boxed{|n_\alpha\rangle = \frac{1}{\sqrt{n_\alpha!}} \left(a_\alpha^\dagger\right)^{n_\alpha} |0\rangle}$$

$a_\alpha^\dagger$ raises the occupation # n_α by +1.

— creation operator

Similarly a_α lowers it ($\Rightarrow$ annihilation operator)

$$a_\alpha |n_\alpha\rangle = \frac{1}{\sqrt{n_\alpha!}} a_\alpha \left(a_\alpha^\dagger\right)^{n_\alpha} |0\rangle$$

$$= \frac{1}{\sqrt{n_\alpha!}} \left(1 + a_\alpha^\dagger a_\alpha\right) \left(a_\alpha^\dagger\right)^{n_\alpha - 1} |0\rangle$$

$$= \frac{1}{\sqrt{n_\alpha}} \left(1 + \hat{n}_\alpha\right) |n_\alpha - 1\rangle = \sqrt{n_\alpha}\, |n_\alpha - 1\rangle.$$

$$\boxed{\begin{aligned} a_\alpha |n_\alpha\rangle &= \sqrt{n_\alpha}\, |n_\alpha - 1\rangle \\ a_\alpha^\dagger |n_\alpha\rangle &= \sqrt{1 + n_\alpha}\, |n_\alpha + 1\rangle \end{aligned}}$$

[Comment: Operators with this algebra are presumably familiar from QM of SHO.

An explicit representation is to write

$$a = \frac{x + ip}{\sqrt{2}}, \quad a^\dagger = \frac{x - ip}{\sqrt{2}} \quad \text{with } [x, p] = i$$

Then $a^\dagger a = \frac{1}{2}(x^2 + p^2) - \frac{1}{2}$ which has

eigenvalues n = integer in $[0, \infty)$.]

For fermions the occupation # $n_\alpha = 0$ or 1 for each α.

So now introduce operators that satisfy the algebra

$$\{a_\alpha, a_\alpha^\dagger\} = 1 \quad \text{where } \{A, B\} = AB + BA$$

= anticommutator

with $a_\alpha |0_\alpha\rangle = 0$, and $a_\alpha^2 = a_\alpha^{\dagger 2} = 0$.

Then define $|1_\alpha\rangle = a_\alpha^\dagger |0_\alpha\rangle$

$$(a_\alpha^\dagger a_\alpha)|1_\alpha\rangle = a_\alpha^\dagger a_\alpha a_\alpha^\dagger |0_\alpha\rangle = a_\alpha^\dagger (1 - a_\alpha^\dagger a_\alpha)|0_\alpha\rangle$$

$$= a_\alpha^\dagger |0_\alpha\rangle = |1_\alpha\rangle$$

$\therefore$ $|1_\alpha\rangle$ is an eigenstate of $\hat{n}_\alpha = a_\alpha^\dagger a_\alpha$ with eigenvalue 1.

Consider $a^\dagger_\alpha |1_\alpha\rangle = (a^\dagger_\alpha)^2 |0_\alpha\rangle = 0$.

$\therefore$ There are only 2 states $|0_\alpha\rangle$ and $|1_\alpha\rangle$ as required.

$$a^\dagger_\alpha |0_\alpha\rangle = |1_\alpha\rangle$$

$$\text{and} \quad a_\alpha |1_\alpha\rangle = |0_\alpha\rangle .$$

Now consider a many particle system where many single particle states can be occupied.

For bosons, impose commutation relations between $(a_\alpha, a^\dagger_\alpha)$ operators at different α, i.e let

$$[a_\alpha, a^\dagger_{\alpha'}] = \delta_{\alpha\alpha'}, \quad [a_\alpha, a_{\alpha'}] = [a^\dagger_\alpha, a^\dagger_{\alpha'}] = 0.$$

For fermions, let $\{a_\alpha, a^\dagger_{\alpha'}\} = \delta_{\alpha\alpha'}$

$$\{a_\alpha, a_{\alpha'}\} = \{a^\dagger_\alpha, a^\dagger_{\alpha'}\} = 0.$$

Define the <u>vaccuum</u> to be the state with no particles so that every $n_\alpha = 0$.

Denote this state $|0\rangle$

$$\forall \alpha \, , \quad a_\alpha |0\rangle = 0 .$$

A general state $|\{n_\alpha\}\rangle$ may then be written

$$\boxed{|\{n_\alpha\}\rangle = \frac{1}{\sqrt{\prod_\alpha (n_\alpha !)}} \prod_\alpha \left(a_\alpha^\dagger\right)^{n_\alpha} |0\rangle}$$ ~~for bosons~~

$$\cancel{= \prod_\alpha \left(a_\alpha^\dagger\right)^{n_\alpha} |0\rangle \text{ for fermions}} ,$$

Note : Due to the (anti) commutation relations, this state is automatically (anti) symmetrized and hence is in the correct Hilbert space for (fermions) bosons.

To go from creation/ann. operators in the $\{|\alpha\rangle\}$ basis to any other basis is straightforward (usual unitary transformation).

Often the position basis is convenient.

Define $\hat{\psi}(x) = \sum_\alpha \phi_\alpha(x)\,\hat{a}_\alpha$

$$\hat{\psi}^\dagger(x) = \sum_\alpha \phi^*_\alpha(x)\,\hat{a}^\dagger_\alpha$$

where $\phi_\alpha(x)$ is the wave function of the state $|\alpha\rangle$.

Then (for bosons) $\left[\hat{\psi}(x), \hat{\psi}^\dagger(x')\right] = \delta(x-x')$

$$\left[\hat{\psi}(x), \hat{\psi}(x')\right] = \left[\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x')\right] = 0$$

For fermions $\left\{\hat{\psi}(x), \hat{\psi}^\dagger(x')\right\} = \delta(x-x')$

$$\left\{\hat{\psi}(x), \hat{\psi}(x')\right\} = \left\{\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x')\right\} = 0.$$

These are known as "field operators".

The creation/annihilation operators provide an extremely useful language for discussing many body problems ..

All physical operators may be written in terms of these operators.

Consider first "1-body" operators

$$\hat{V} = \begin{cases} \sum_i V(x_i) \\ \sum_i f_1(x_i, \partial/\partial x_i) \end{cases}$$

etc

which are the sums of several operators each one of which acts only on one particle.

(Eg: Kinetic energy operator $\hat{T} = \sum_i \vec{p}_i^{\,2}/2m$).

Go to a ~~basis~~ single particle basis in which $\hat{V}_1$ is diagonal:

(Negele/Orland: Pages 16-19)

$$\hat{V}_1 |\alpha\rangle = V_{1\alpha} |\alpha\rangle .$$

$$V_{1\alpha} = \langle\alpha|\hat{V}_1|\alpha\rangle \, .$$

For a many body state $|\{n_\alpha\}\rangle$ it is physically obvious that $\hat{V} = \sum_{\cancel{\alpha}} \hat{V}_{1i}$

$$= \sum_\alpha V_{1\alpha} \hat{n}_\alpha$$

$$= \sum_\alpha \langle\alpha|\hat{V}_1|\alpha\rangle a^\dagger_\alpha a_\alpha$$

In a general basis $|\mu\rangle$,

$$a_{\alpha} = \sum_{\mu} \langle\alpha|\mu\rangle a_\mu$$

$$a^\dagger_\alpha = \sum_{\lambda} \langle\lambda|\alpha\rangle a^\dagger_\lambda$$

$$a^\dagger_\alpha a_\alpha = \sum_{\mu\lambda} \langle\alpha|\mu\rangle\langle\lambda|\alpha\rangle a^\dagger_\lambda a_\mu$$

$$\hat{V} = \sum_{\alpha\lambda,\mu} V_{1\alpha} \langle\lambda|\alpha\rangle\langle\alpha|\mu\rangle a^\dagger_\lambda a_\mu$$

$$= \sum_{\lambda\mu} \langle\lambda|\hat{V}_1|\mu\rangle a^\dagger_\lambda a_\mu \equiv \sum_{\lambda\mu} V_{\lambda\mu} a^\dagger_\lambda a_\mu$$

~~For d~~

Example: In position basis

$$\langle \lambda | V_1 | \mu \rangle = \int d^d x \, d^d y \; \phi^*_\lambda(x) \, \phi_\mu(y) \langle x | U | y \rangle$$

where $\phi_\lambda(x)$ are the wavefunctions of state λ.

(i) A potential term $\hat{V} = \sum_i V(x_i)$

$V(x_i)$ is diagonal in the position basis.

$$\therefore \hat{V} = \int d^3x \; V(x) \, \psi^\dagger(x) \, \psi(x)$$

Note that $\psi^\dagger(x) \psi(x)$ is the density operator.

(ii) Kinetic operator $\hat{T} = \sum_i \hat{p}_i^2 / 2m = \sum_i \frac{1}{2m} \left(-\nabla_i^2 \right)$

$\therefore$ In 2nd quantized form

$$\hat{T} = \int d^d x \; \psi^\dagger(x) \left(-\frac{\nabla^2}{2m} \right) \psi(x)$$

$$= \int \frac{d^d p}{(2\pi)^d} \left(a^\dagger(p) \, a(p) \right) p^2 / 2m$$

The ~~2nd equation~~ is ~~obvious~~

Consider a large but finite system of volume V (or more specifically a cubic box of volume V)

~~Then allowed set of momenta are (assuming periodic~~ boundary condition) $\vec{p} = \frac{2\pi}{L}\vec{n}$

where $\vec{n} = (n_1, n_2, \ldots)$ is a vector with integer entries.

~~The kinetic operator is diagonal in this $\vec{p}$-basis~~

$$\hat{T} = \sum_{\vec{p}} \frac{\vec{p}^2}{2m} a_p^+ a_p .$$

To go to the position basis, use

$$\hat{\psi}(x) = \sum_{\vec{p}} \langle \vec{x} | \vec{p} \rangle a_p = \frac{1}{\sqrt{V}} \sum_{\vec{p}} e^{i\vec{p}\cdot\vec{x}} a_p$$

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

Conversely $a_p = \frac{1}{\sqrt{V}} \int d^3x \; e^{-i\vec{p}\cdot\vec{x}} \hat{\psi}(x)$

$$a_p^\dagger = \frac{1}{\sqrt{V}} \int d^3x \; e^{i\vec{p}\cdot\vec{x}} \hat{\psi}^\dagger(x) .$$

[Note: Explicitly check that $[\psi(x), \psi^\dagger(x')] = \delta(x-x')$, etc]

$$\hat{T} = \frac{1}{V} \int d^3x \, d^3x' \sum_p \frac{\vec{p}^{\,2}}{2m} e^{i\vec{p}\cdot(\vec{x}-\vec{x}')} \psi^\dagger(x)\psi(x')$$

$$= \frac{1}{V} \int d^3x \, d^3x' \sum_p \left(\frac{-\nabla'^2}{2m}\right) e^{i\vec{p}\cdot(\vec{x}-\vec{x}')} \psi^\dagger(x)\psi(x')$$

$$= \frac{1}{V} \int d^3x \, d^3x' \sum_p e^{i\vec{p}\cdot(\vec{x}-\vec{x}')} \psi^\dagger(x)\left(\frac{-\nabla'^2}{2m}\right)\psi(x')$$

$$= \int d^3x \, d^3x' \, \delta(\vec{x}-\vec{x}') \, \psi^\dagger(x)\left(\frac{-\nabla'^2}{2m}\right)\psi(x')$$

$$= \int d^3x \;\; \psi^\dagger(x)\left(\frac{-\nabla^2}{2m}\right)\psi(x)$$

as expected.

Now consider "two-body" operators

$$\hat{V} = \sum_{i,j} V_2(x_i, x_j), \quad \text{etc.},$$

Eg: $\hat{V} = \sum_{i,j} \frac{K}{|x_i - x_j|^\alpha}$ which is a 2-body interaction.

Again go to a basis in which V_2 is diagonal:

$$\hat{V}_2 |\alpha\beta\rangle = V_{\alpha\beta} |\alpha\beta\rangle$$

$$V_{\alpha\beta} = \langle \alpha\beta | V_2 | \alpha\beta \rangle$$

Then for a general many-particle state $|\{n_\alpha\}\rangle$,

$$\hat{V} = \frac{1}{2} \sum_{\alpha\beta} V_{\alpha\beta} \hat{P}_{\alpha\beta}$$

where $\hat{P}_{\alpha\beta}$ counts # of pairs of particles in the states $|\alpha\rangle$ and $|\beta\rangle$.

(The $1/2$ is to avoid double counting as we sum over both (α,β) and (β,α)).

$$\hat{P}_{\alpha\beta} = \hat{n}_\alpha \hat{n}_\beta \quad \text{if } \alpha \text{ \& } \beta \text{ are distinct}$$

$$= \hat{n}_\alpha(\hat{n}_\alpha - 1) \quad \text{if } \alpha \text{ \& } \beta \text{ are the same}$$

$$\Rightarrow \hat{P}_{\alpha\beta} = \hat{n}_\alpha \hat{n}_\beta - \hat{n}_\alpha \delta_{\alpha\beta}$$

$$= a^\dagger_\alpha a_\alpha a^\dagger_\beta a_\beta - a^\dagger_\alpha a_\alpha \delta_{\alpha\beta}$$

$$= a^\dagger_\alpha \left(\delta_{\alpha\beta} + \xi a^\dagger_\beta a_\alpha\right) a_\beta - a^\dagger_\alpha a_\alpha \delta_{\alpha\beta}$$

($\xi = +1$ for bosons, $= -1$ for fermions).

$$\therefore \hat{P}_{\alpha\beta} = \xi a^\dagger_\alpha a^\dagger_\beta a_\alpha a_\beta = a^\dagger_\alpha a^\dagger_\beta a_\beta a_\alpha$$

$$\boxed{\therefore \hat{V} = \frac{1}{2} \sum_{\alpha\beta} V_{\alpha\beta} \hat{P}_{\alpha\beta} = \frac{1}{2} \sum_{\alpha\beta} \langle \alpha\beta | \hat{V}_2 | \alpha\beta \rangle \, a^\dagger_\alpha a^\dagger_\beta a_\beta a_\alpha .}$$

Transforming from the diagonal basis to an arbitrary basis as before

$$\cancel{\hat{V} = \frac{1}{2} \sum_{\lambda\mu\nu\rho} \langle \{\lambda\mu\} | \hat{V} | \{\nu\rho\} \rangle a^+_\lambda a^+_\mu a_\rho a_\nu}$$

$$\hat{V} = {}^1\!/_2 \sum_{\lambda\mu\nu\rho} \langle \lambda\mu | \hat{V} | \nu\rho \rangle a^+_\lambda a^+_\mu a_\rho a_\nu$$

<u>Example</u>: If $\hat{V} = \sum_{i,j} V(x_i, x_j)$ which is diagonal in the x-basis

in 2nd quantization

$$\hat{V} = \int d^3x \, d^3x' \left(\psi^+(x) \psi^+(x') \psi(x') \psi(x) \right) V(\vec{x}, \vec{x}')$$

$$= \sum_{p_1, p_2, p_3, p_4} \left(a^+_{p_1} a^+_{p_2} a_{p_4} a_{p_3} \right) \langle p_1 p_2 | V | p_3 p_4 \rangle$$

where $\langle p_1 \, p_2 | V | p_3 \, p_4 \rangle = \int d^dx \, d^dx' \; e^{-i(\vec{p}_1 + \vec{p}_2) \cdot \vec{x}}$
$V(\vec{x}, \vec{x}') \; e^{+i(\vec{p}_3 + \vec{p}_4) \cdot \vec{x}'}$

Can similarly generalize to n-body operators.

[Comment: It is useful to consider an enlarged Hilbert space ~~in~~ which allows for states with arbitrary total # of particles N. Formally consider the direct sum of the Hilbert spaces of particle # N with N running from 0 to ∞. This enlarged space is called Fock space. The operators a & $a^\dagger$ act on states in Fock space as they change the total particle #.]

We can now write any many body Hamiltonian in 2^{nd} quantized form.

Examples

(1) Consider ~~spinless particles~~ bosons in a harmonic trap with short ranged repulsive interactions

$$H = \sum_{i=1}^{N} \vec{p}_i^{\,2}/2m + \frac{1}{2} m\omega^2 \sum_i \vec{x}_i^{\,2} + \sum_{i<j} U(\vec{r}_i - \vec{r}_j)$$

In 2^{nd} quantized notation

$$H = \int d^d x \; \psi^\dagger(x) \left(-\frac{\nabla^2}{2m} + \frac{1}{2} m\omega^2 x^2 \right) \psi(x)$$

$$+ \frac{1}{2} \int d^d x \, d^d x' \; U(\vec{x} - \vec{x}') \, \psi^\dagger(x) \psi^\dagger(x') \psi(x') \psi(x).$$

(2) We may generalize above to spin-s fermions ($s = \frac{1}{2}$(integer)).

Field operators will carry a spin index

$$\psi_\sigma(x) \quad \text{with} \quad \sigma = -s, \ldots, s \quad (= 2s+1 \text{ values})$$

$$\{\psi_\sigma(x), \psi^\dagger_{\sigma'}(x')\} = \delta_{\sigma\sigma'}\,\delta(x-x')$$

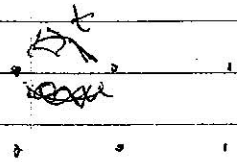
$$\{\psi_\sigma(x), \psi_{\sigma'}(x')\} = \{\psi^\dagger_\sigma(x), \psi^\dagger_{\sigma'}(x')\} = 0.$$

$$H = \int d^d x \sum_\sigma \psi^\dagger_\sigma(x)\left(-\frac{\nabla^2}{2m} + \frac{1}{2}m\omega^2 x^2\right)\psi_\sigma(x)$$

$$+\frac{1}{2}\int d^d x\, d^d x'\; U(x-x')\,\psi^\dagger_\sigma(x)\,\psi^\dagger_{\sigma'}(x')\,\psi_{\sigma'}(x')\,\psi_\sigma(x).$$

(3) Tight binding model of electrons in a solid:

Electrons taken to live on the sites of some lattice.



Eg: $d = 2$ square lattice.

If the electron is on site i, energy $= \epsilon_i$

Amplitude $-t$ to hop to nearest neighbour sites.

Introduce $a_{i\alpha}$ = destruction operator for electron of spin α at site i

& llly $a^\dagger_{i\alpha}$.

$$\{a_{i\alpha}, a^\dagger_{j\alpha'}\} = \delta_{\alpha\alpha'}\delta_{ij}$$

$$\{a_{i\alpha}, a_{j\beta}\} = \{a^\dagger_{i\alpha}, a^\dagger_{j\beta}\} = 0$$

$$H = \sum_i \epsilon_i a^\dagger_{i\alpha} a_{i\alpha} - \sum_{\langle ij\rangle} t_{ij} \left(a^\dagger_{i\alpha} a_{j\alpha} + h.c\right).$$

Sometimes useful to include a chemical potential in the Hamiltonian (i.e consider $H' = H - \mu N$ instead of H).

$$H' = \sum_i (\epsilon_i - \mu) a^\dagger_{i\alpha} a_{i\alpha} - \sum_{\langle ij\rangle} t_{ij} \left(a^\dagger_{i\alpha} a_{j\alpha} + h.c\right)$$

4 Consider $\epsilon_i = 0$.

Assume that if two electrons are at same site, there is repulsion U ($\Rightarrow$ 2-body interaction)

$$H = -\sum_{\langle ij \rangle} t_{ij} \left(a^{+}_{i\alpha} a_{j\alpha} + h.c \right) - \mu \sum_{i\alpha} \hat{n}_{i\alpha}$$

$$+ U \sum_{i} \hat{n}_i \frac{(\hat{n}_i - 1)}{2}$$

$\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$ = total electron # at each site.

This is known as the Hubbard model.

Comments: 1 Writing the Hamiltonian in 2^{nd} quantization is not a solution to the problem but is just a language to pose the problem.

2 It is useful to be able to go back & forth between 1^{st} quantized & 2^{nd} quantized formulations of the problem.

A priori for any new many body problem, it is not clear that which formulation is clearly better.

There are great examples for the success of either formulation

Eg: Superconductivity was explained by BCS by using the 2^{nd} quantized formulation & guessing a good variational 2^{nd} quantized wavefunction for the ground state. The 1^{st} quantized formulation - while also providing some insight - is more cumbersome.

On the other hand the FQHE was explained by Laughlin by working in 1^{st} quantization, and guessing a good variational 1^{st} quantized wave function for the ground state. Here the 2^{nd} quantized approach came later!

It is often also useful to adopt a path integral formulation of the quantum problem