Second Quantization

Jan von Delft, 17.11.2020

Motivation: to simplify treatment of exchange symmetry in many-particle systems

$$H = \underbrace{\sum_i \varepsilon_i c_i^\dagger c_i}_{\text{on-site energy}} + \underbrace{\sum_{ij} t(c_i^\dagger c_j + c_j^\dagger c_i)}_{\text{hopping between sites i and j}} + \underbrace{\sum_{ij} V_{ij}\, c_i^\dagger c_i c_j^\dagger c_j}_{\text{interaction between sites i and}}$$

$$[c_i, c_j^\dagger]_\zeta = \delta_{ij}, \quad [c_i, c_j]_\zeta = 0, \quad [c_i^\dagger, c_j^\dagger]_\zeta = 0,$$

$$[A, B]_\zeta = AB + \zeta BA, \quad \zeta = \pm 1 \quad \text{for} \begin{cases} \text{bosons} \\ \text{fermions} \end{cases}$$

Assumed background:
elementary quantum mechanics, Dirac bra-ket notation, Bose and Fermi statistics

Literature: numerous textbooks on many-body physics have an introductory chapter or an appendix on 2nd quantization. Examples (these notes follow Altland & Simons):

- A. Altland & B. Simons, Condensed Matter Field Theory, Cambridge University Press, 2nd Ed. (2010), Sec.2.1-2
- A. L. Fetter & J. D. Walecka, Quantum Theory of Many-Particle Systems, McGraw-Hill (1971), Chapter 1.
- G. Rickayzen, Greens Functions and Condensed Matter Physics, Dover (2013), Appendix A
- S. M. Girvin & K. Yang, Modern Condensed Matter Physics, Cambridge University Press (2019), Appendix J.

Single-particle basis

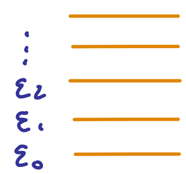
Consider a single-particle quantum system.

Single-particle Hilbert space: $\mathcal{H}_{(1)} = \text{span}\{ |\lambda\rangle \mid \text{all values of } \lambda \}$ (1)

Wavefunction: $(x \in \mathbb{R}^d)$ $\psi_\lambda(x) = \langle x | \lambda \rangle$ (2)

It is often convenient (though not necessary) to choose the basis states to be eigenstates of a single-particle Hamiltonian: $\hat{H}_{(1)}(\hat{r}, \hat{p})$ (3)

Eigenvalue equation: $\hat{H}_{(1)} |\lambda\rangle = \varepsilon_\lambda |\lambda\rangle$ (4)



Having this example in mind, we will assume that the λ label takes the values $0, 1, 2, \ldots$

Example: harmonic oscillator: $\hat{H}_{(1)}(\hat{r}, \hat{p}) = \frac{1}{2m}\hat{p}^2 + \frac{1}{2} m \omega^2 \hat{x}^2$ (5)

$$\varepsilon_\lambda = (\lambda + \tfrac{1}{2})\hbar\omega, \quad \lambda \in \mathbb{N}_0 \tag{6}$$

In general, λ can also be a continuous index. E.g. for free particles, $\hat{H}_{(1)} = \frac{1}{2m}\hat{p}^2$, $\lambda \leftrightarrow \vec{p}$ (7)

Or, λ can enumerate sites in a lattice, then it is a discrete index, $\lambda \leftrightarrow i \in \mathbb{Z}^d$ (8)

All we need (later) is some ordering convention for its values.

Exchange symmetry: 2 particles

Consider a system of 2 identical particles, described by $\hat{H}_{(2)} = \hat{H}(\hat{x}_1, \hat{p}_1 ; \hat{x}_2, \hat{p}_2)$ (1)

2-particle Hilbert space: $\mathcal{H}_{(2)} = \mathcal{H}_{(1)} \otimes \mathcal{H}_{(1)} = \text{span}\{ |\lambda\rangle \otimes |\lambda'\rangle \}$ (2)

$|\lambda\rangle \otimes |\lambda'\rangle$: 'first' particle in state λ , 'second' particle in state λ' (3a)

$|\lambda'\rangle \otimes |\lambda\rangle$: 'first' particle in state λ' , 'second' particle in state λ (3b)

But particles are <u>indistinguishable</u>, states (3a), (3b) don't have independent physical meaning.

Physically meaningful states must be fully symmetric (bosons) or anti-symmetric (fermions):

Meaningful state: $|\Psi\rangle = \frac{1}{\sqrt{2}} \left[|\lambda\rangle \otimes |\lambda'\rangle + \zeta \, |\lambda'\rangle \otimes |\lambda\rangle \right]$, $\quad \zeta = \pm 1$ for $\left\{ \begin{array}{l} \text{bosons} \\ \text{fermions} \end{array} \right.$ (4)

Wavefunction: $\Psi(x_1, x_2) = \langle x_1 | \otimes \langle x_2 | \Psi\rangle = \frac{1}{\sqrt{2}} \left[\psi_\lambda(x_1) \, \psi_{\lambda'}(x_2) + \zeta \, \psi_{\lambda'}(x_1) \psi_\lambda(x_2) \right]$ (5)

'Exchange symmetry': $\Psi(x_2, x_1) = \zeta \Psi(x_1, x_2)$ invariant up to a sign under $x_1 \leftrightarrow x_2$ (6)

Physical part of 2-particle Hilbert space contains only symmetrized/antisymmetrized states:

2-particle 'Fock space': $\mathcal{F}_{(2)} = \text{span}\{ |\lambda\rangle \otimes |\lambda'\rangle + \zeta \, |\lambda'\rangle \otimes |\lambda\rangle \}$ (7)

Exchange symmetry: N particles

N-particle Hamiltonian: $\hat{H}_{(N)} = \hat{H}(\hat{x}_1, \hat{p}_1 ; \hat{x}_2, \hat{p}_2 ; \cdots ; \hat{x}_N, \hat{p}_N)$ (1)

N-particle Hilbert space: $\mathcal{H}_{(1)}^{\otimes N} = \underbrace{\mathcal{H}_{(1)} \otimes \mathcal{H}_{(1)} \otimes \cdots \otimes \mathcal{H}_{(1)}}_{\text{N copies}} = \text{span}\{ |\lambda_1\rangle \otimes |\lambda_2\rangle \otimes \cdots \otimes |\lambda_N\rangle \}$ (2)

Physical part of this space contains only <u>fully</u> symmetrized/antisymmetrized states of the form:

$$\boxed{\underbrace{|\lambda_1, \lambda_2, \ldots, \lambda_N\rangle}_{\substack{\text{these states are occupied,} \\ \text{all others empty}}} = \mathcal{N} \sum_P \zeta_P \, |\lambda_{P_1}\rangle \otimes |\lambda_{P_2}\rangle \otimes \cdots \otimes |\lambda_{P_3}\rangle} \tag{3}$$

(4)

Sum: over all permutations of N indices. E.g. $P = (P_1 P_2 P_3) \in \{(123), (132), (213), (231), (312), (321)\}$

$\text{sgn}(P)$: $+ \quad - \quad - \quad + \quad + \quad -$

Sign: for bosons: $\zeta_P = 1$ (5)

for fermions $\zeta_P = \text{sgn}(P) = \pm 1$ $\left\{ \begin{array}{l} \text{if even/odd number of transpostions are} \\ \text{needed to convert } (12\ldots N) \text{ to } (P_1 P_2 \ldots P_N) \end{array} \right.$

Normalization $\mathcal{N}$: chosen such that $\langle \lambda_1, \ldots, \lambda_N | \lambda_1, \ldots, \lambda_N\rangle = 1$ (6)

N-particle Fock space: $\mathcal{F}_{(N)} = \text{span}\{ |\lambda_1, \lambda_2, \ldots, \lambda_N\rangle \mid \text{all values of } \{\lambda_j\} \}$ (7)

N-particle wave functions

N-particle position eigenstate: $|x_1, x_2, \dots, x_N\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \dots |x_N\rangle.$ (1)

$$\hat{x}_i |x_1, x_2, \dots, x_N\rangle = x_i |x_1, x_2, \dots, x_N\rangle \quad (2)$$

position operator in i-th single-particle Hilbert space

eigenvalue

N-particle wavefunction: $\langle x_1, x_2, \dots, x_N | \lambda_1, \lambda_2, \dots, \lambda_N\rangle \overset{(4.3)}{=} \mathcal{N} \sum_P \zeta_P \, \psi_{\lambda_{P_1}}(x_1)\, \psi_{\lambda_{P_2}}(x_2) \dots \psi_{\lambda_{P_N}}(x_N)$ (3)

'Exchange symmetry': $\langle \dots, x_i, \dots, x_{i'}, \dots | \{\lambda_j\}\rangle \overset{(3)}{=} \zeta \langle \dots, x_{i'}, \dots, x_i, \dots | \{\lambda_j\}\rangle$ (4)

For fermions, wavefunction is a determinant:

'Slater determinant'

$$\langle \{x_i\} | \{\lambda_j\}\rangle \overset{\text{fermions}}{=} \mathcal{N} \begin{vmatrix} \psi_{\lambda_1}(x_1) & \psi_{\lambda_2}(x_1) & \dots & \psi_{\lambda_N}(x_1) \\ \psi_{\lambda_1}(x_2) & \psi_{\lambda_2}(x_2) & & \vdots \\ \vdots & & \ddots & \\ \psi_{\lambda_1}(x_N) & \dots & & \psi_{\lambda_N}(x_N) \end{vmatrix} \quad (5)$$

Antisymmetry of determinant under exchange of rows or columns implies:

$\langle \{x_i\} | \{\lambda_j\}\rangle \overset{(5)}{=} 0$ if $\left\{ \begin{array}{lll} \lambda_j = \lambda_{j'} & \text{two particles in same state} \\ x_i = x_{i'} & \text{two particles at same position} \end{array} \right\}$ 'Pauli exclusion principle' (6)

N-particle basis: occupation number representation

Due to exchange symmetry, we can fully specify a basis state

$$\boxed{|\lambda_1, \lambda_2, \dots, \lambda_N\rangle = \mathcal{N} \sum_P \zeta_P |\lambda_{P_1}\rangle \otimes |\lambda_{P_2}\rangle \otimes \dots \otimes |\lambda_{P_3}\rangle = |n_0, n_1, n_2, \dots\rangle} \quad (1)$$

by specifying how many particles, n_λ, populate each $|\lambda\rangle$, with $\sum_\lambda n_\lambda = N$. (2)

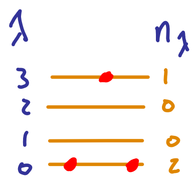
For 'bosons', $n_\lambda \in \mathbb{N}_0$: each $|\lambda\rangle$ can contain arbitrarily many bosons. (3)

For 'fermions', $n_\lambda \in \{0, 1\}$: each $|\lambda\rangle$ can contain at most one fermion ('Pauli principle') (4)

Examples: the states on the right are denoted as

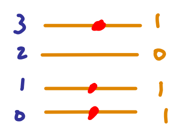
λ_j representation $\qquad$ n_λ representation

$|\lambda_1 = 0, \lambda_2 = 0, \lambda_3 = 3\rangle = |n_0 = 2, n_1 = 0, n_2 = 0, n_3 = 1, n_4 = 0, \dots\rangle$ (5)



3 bosons

$|\lambda_1 = 0, \lambda_2 = 1, \lambda_3 = 3\rangle = |n_0 = 1, n_1 = 1, n_2 = 0, n_3 = 1, n_4 = 0, \dots\rangle$ (6)



3 fermions

Fock space, creation operators

N-particle Fock space: $\mathcal{F}_{(N)} = \mathrm{span}\left\{ |n_0, n_1, n_2, \dots\rangle \,\middle|\, n_i \in \left\{\begin{matrix} \mathbb{N}_0 \\ \{0,1\} \end{matrix}\right\}, \sum_\lambda n_\lambda = N \right\}$ (bosons / fermions) (1)

It is often convenient to not impose the condition of fixed particle number N. Then consider

(many-particle) Fock space: $$\boxed{\mathcal{F} = \sum_{\oplus N}^{\infty} \mathcal{F}_{(N)} = \mathrm{span}\{|n_0, n_1, n_2, \dots\rangle\}}$$ total particle number not fixed (2)

'Vacuum space': $$\boxed{\mathcal{F}_{(0)} = \mathrm{span}\{|\Omega\rangle\}, \quad |\Omega\rangle = |0,0,0,\dots\rangle}$$ 'vacuum state' (3)

Define 'creation operators' connecting states which differ by 1 for specified occupation number:

$$\boxed{a^\dagger_\lambda |n_0, \dots, n_\lambda, \dots\rangle = (n_\lambda + 1)^{1/2} \zeta^{s_\lambda} |n_0, \dots, n_\lambda + 1, \dots\rangle,} \quad (4)$$

creates particle in state λ

'fermionic sign' depends on how many 'earlier' states are occupied: $$s_\lambda = \sum_{\tilde\lambda = 0}^{\lambda - 1} n_{\tilde\lambda} \quad (5)$$

For fermions, occupation numbers are defined modulo 2, i.e. $(1+1) \bmod 2 = 0$

so, $$a^\dagger_\lambda |n_0, \dots, n_\lambda = 1, \dots\rangle \propto \left((1+1) \bmod 2\right)^{1/2} = 0$$ [this encodes Pauli principle (6.4)] (6)

All states can be obtained from vacuum state by repeated action of $a^\dagger$'s: $$\boxed{|n_0, n_1, n_2, \dots\rangle = \mathcal{N} (a^\dagger_0)^{n_0} (a^\dagger_1)^{n_1} (a^\dagger_2)^{n_2} \dots |\Omega\rangle} \quad (7)$$

(Anti)-commutation relations $[a^\dagger, a^\dagger]$

Def: $[A, B]_\zeta \equiv AB - \zeta BA = \begin{cases} AB - BA = [A,B] & \text{= commutator, for bosons} \quad (1a) \\ AB + BA = \{A,B\} & \text{= anti-commutator, for fermions} \quad (1b) \end{cases}$

Claim: creation operators satisfy $$\boxed{[a^\dagger_\lambda, a^\dagger_{\lambda'}]_\zeta = 0} \quad (2)$$

$s_\lambda = \sum_{\tilde\lambda=0}^{\lambda-1} n_{\tilde\lambda}$

Proof:

- Equal indices, $\lambda = \lambda'$: For bosons, $a^\dagger_\lambda a^\dagger_\lambda - a^\dagger_\lambda a^\dagger_\lambda = 0$ (trivially true) (3)

For fermions: $a^\dagger_\lambda a^\dagger_\lambda |\dots, n_\lambda = 0, \dots\rangle = a^\dagger_\lambda \zeta^{s_\lambda} 1 \cdot |\dots, n_\lambda = 1, \dots\rangle \overset{(7.6)}{=} 0$ (4)

This holds for all states in $\mathcal{F}$, hence $a^\dagger_\lambda a^\dagger_\lambda = 0$, and also $a^\dagger_\lambda a^\dagger_\lambda + a^\dagger_\lambda a^\dagger_\lambda = 0$ (5)

- Unequal indices, $\lambda \neq \lambda'$:

Simplest example: action on vacuum state, $|\Omega\rangle = |n_0 = 0, n_1 = 0, n_2 = 0, \dots\rangle$: (6)

$$a^\dagger_1 a^\dagger_0 |0,0,0,0,\dots\rangle \overset{(7.4)}{=} a^\dagger_1 \zeta^0 |1,0,0,0,\dots\rangle \overset{(7.4)}{=} \zeta^1 |1,1,0,0,\dots\rangle \quad (7)$$

$$a^\dagger_0 a^\dagger_1 |0,0,0,0,\dots\rangle \overset{(7.4)}{=} a^\dagger_0 \zeta^0 |0,1,0,0,\dots\rangle \overset{(7.4)}{=} \zeta^0 |1,1,0,0,\dots\rangle \quad (8)$$

$$\Longrightarrow \quad (a^\dagger_1 a^\dagger_0 - \zeta a^\dagger_0 a^\dagger_1) |0,0,0,0,\dots\rangle = 0 \quad (9)$$

General case: assume (without loss of generality) $\lambda < \lambda'$: $\quad s_\lambda = \sum_{\tilde{\lambda}=0}^{\lambda-1} n_{\tilde{\lambda}}$

$$a^\dagger_\lambda a^\dagger_{\lambda'} |\dots, n_\lambda, \dots, n_{\lambda'}, \dots\rangle = (n_{\lambda'}+1)^{1/2} a^\dagger_\lambda \, \zeta^{s_{\lambda'}} |\dots, n_\lambda, \dots, n_{\lambda'}+1, \dots\rangle \tag{1}$$

$$= (n_\lambda+1)^{1/2}(n_{\lambda'}+1)^{1/2} \zeta^{s_\lambda} \zeta^{s_{\lambda'}} |\dots, n_\lambda+1, \dots, n_{\lambda'}+1, \dots\rangle \tag{2}$$

$$a^\dagger_{\lambda'} a^\dagger_\lambda |\dots, n_\lambda, \dots, n_{\lambda'}, \dots\rangle = (n_\lambda+1)^{1/2} a^\dagger_{\lambda'} \, \zeta^{s_\lambda} |\dots, n_\lambda+1, \dots, n_{\lambda'}, \dots\rangle \tag{3}$$

$$= (n_{\lambda'}+1)^{1/2}(n_\lambda+1)^{1/2} \zeta \, \zeta^{s_{\lambda'}} \zeta^{s_\lambda} |\dots, n_\lambda+1, \dots, n_{\lambda'}+1, \dots\rangle \tag{4}$$

$$\left(a^\dagger_\lambda a^\dagger_{\lambda'} - \zeta \, a^\dagger_{\lambda'} a^\dagger_\lambda\right) |\dots, n_\lambda, \dots, n_{\lambda'}, \dots\rangle \overset{(2,4)}{=} 0 \tag{5}$$

(5) holds for <u>all</u> basis kets $|\dots, n_\lambda, \dots, n_{\lambda'}, \dots\rangle$ of $\mathcal{F}$, hence it is an operator identity:

$$\boxed{[a^\dagger_\lambda, a^\dagger_{\lambda'}]_\zeta = a^\dagger_\lambda a^\dagger_{\lambda'} - \zeta \, a^\dagger_{\lambda'} a^\dagger_\lambda = 0} \tag{6}$$

'boson creation operators commute, fermion creation operators anti-commute'

<u>(Anti)-commutation relations</u> $[a, a]$

Recall definition of creation operator: $a^\dagger_\lambda |n'_0, \dots, n'_\lambda, \dots\rangle = (n'_\lambda+1)^{1/2} \zeta^{s_\lambda} |n'_0, \dots, n'_\lambda+1, \dots\rangle$ (1)

Matrix elements: $\langle n_0, \dots, n_\lambda, \dots | a^\dagger_\lambda | n'_0, \dots, n'_\lambda, \dots\rangle = (n'_\lambda+1)^{1/2} \zeta^{s_\lambda} \, \delta_{n_0, n'_0} \dots \delta_{n_\lambda, n'_\lambda+1} \dots$ (2)

rewrite $\downarrow$ $\quad n_\lambda = n'_\lambda + 1$, $\quad n'_\lambda = n_\lambda - 1$

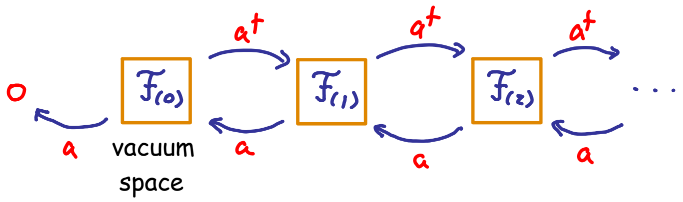
Complex conjugate: $\langle n'_0, \dots, n'_\lambda, \dots | a_\lambda | n_0, \dots, n_\lambda, \dots\rangle = (n_\lambda)^{1/2} \zeta^{s_\lambda} \, \delta_{n'_0, n_0} \dots \delta_{n'_\lambda, n_\lambda - 1} \dots$ (3)

(3) holds for <u>all</u> basis bras $\langle \dots, n'_\lambda, \dots, n'_{\lambda'}, \dots |$ of $\mathcal{F}$, hence we conclude that

$$\boxed{a_\lambda |n_0, \dots, n_\lambda, \dots\rangle = (n_\lambda)^{1/2} \zeta^{s_\lambda} |n_0, \dots, n_\lambda - 1, \dots\rangle} \tag{4}$$

i.e. a_λ 'annihilates' or 'destroys' a particle in state λ.

Action in Fock space: (5)



Hermitian conjugate of (9.6): $\underline{[a_\lambda, a_{\lambda'}]_\zeta = a_\lambda a_{\lambda'} - \zeta \, a_{\lambda'} a_\lambda = 0}$ (6)

(Anti)-commutation relations $[a,a^\dagger]$

Consider equal indices: $\lambda = \lambda'$:

$$a_\lambda a^\dagger_\lambda |\ldots,n_\lambda,\ldots\rangle = a_\lambda (n_\lambda+1)^{1/2}\zeta^{s_\lambda}|\ldots,n_\lambda+1,\ldots\rangle = (n_\lambda+1)^{1/2+\frac{1}{2}}\underbrace{(\zeta^{s_\lambda})^2}_{=1}|\ldots,n_\lambda,\ldots\rangle \qquad (1)$$

$$a^\dagger_\lambda a_\lambda |\ldots,n_\lambda,\ldots\rangle = a^\dagger_\lambda (n_\lambda)^{1/2}\zeta^{s_\lambda}|\ldots,n_\lambda-1,\ldots\rangle = (n_\lambda)^{1/2+1/2}(\zeta^{s_\lambda})^2|\ldots,n_\lambda,\ldots\rangle \qquad (2)$$

Bosons:

$$(a_\lambda a^\dagger_\lambda - a^\dagger_\lambda a_\lambda)|\ldots,n_\lambda,\ldots\rangle \overset{(1,2)}{=} 1\cdot|\ldots,n_\lambda,\ldots\rangle \Rightarrow \boxed{a_\lambda a^\dagger_\lambda - a^\dagger_\lambda a_\lambda = 1} \qquad (3)$$

holds for all basis kets!

Fermions:

$$(a_\lambda a^\dagger_\lambda + a^\dagger_\lambda a_\lambda)|\ldots,n_\lambda=0,\ldots\rangle = (1+0)\,|\ldots,n_\lambda=0,\ldots\rangle = |\ldots,n_\lambda=0,\ldots\rangle \qquad (4)$$

$$(a_\lambda a^\dagger_\lambda + a^\dagger_\lambda a_\lambda)|\ldots,n_\lambda=1,\ldots\rangle = \big((1+1)\,\mathrm{mod}\,2 + 1\big)\,|\ldots,n_\lambda=1,\ldots\rangle = |\ldots,n_\lambda=1,\ldots\rangle \qquad (5)$$

(4,5) hold for all basis kets! $\Rightarrow \boxed{a_\lambda a^\dagger_\lambda + a^\dagger_\lambda a_\lambda = 1}$ (6)

(7)

Compact formulation of (3) & (6): $\boxed{[a_\lambda, a^\dagger_\lambda]_\zeta = 1}$

(Anti)-commutation relations $[a,a^\dagger]$

General case: assume (without loss of generality) $\lambda < \lambda'$ (analogous to p. 9): $s_\lambda = \sum_{\tilde\lambda=0}^{\lambda-1} n_{\tilde\lambda}$

$$a_\lambda a^\dagger_{\lambda'}|\ldots,n_\lambda,\ldots,n_{\lambda'},\ldots\rangle = (n_{\lambda'}+1)^{1/2}\,a_\lambda\,\zeta^{s_{\lambda'}}\,|\ldots,n_\lambda,\ldots,n_{\lambda'}+1,\ldots\rangle \qquad (1)$$

$$= (n_\lambda)^{1/2}(n_{\lambda'}+1)^{1/2}\zeta^{s_\lambda}\zeta^{s_{\lambda'}}|\ldots,n_\lambda-1,\ldots,n_{\lambda'}+1,\ldots\rangle \qquad (2)$$

$$a^\dagger_{\lambda'}a_\lambda|\ldots,n_\lambda,\ldots,n_{\lambda'},\ldots\rangle = (n_\lambda)^{1/2}\,a^\dagger_{\lambda'}\,\zeta^{s_\lambda}\,|\ldots,n_\lambda-1,\ldots,n_{\lambda'},\ldots\rangle \qquad (3)$$

$$= (n_{\lambda'}+1)^{1/2}(n_\lambda)^{1/2}\zeta\,\zeta^{s_{\lambda'}}\zeta^{s_\lambda}|\ldots,n_\lambda-1,\ldots,n_{\lambda'}+1,\ldots\rangle \qquad (4)$$

$$(a_\lambda a^\dagger_{\lambda'} - \zeta\, a^\dagger_{\lambda'}a_\lambda)|\ldots,n_\lambda,\ldots,n_{\lambda'},\ldots\rangle \overset{(2,4)}{=} 0 \Rightarrow \boxed{a_\lambda a^\dagger_{\lambda'} - \zeta\, a^\dagger_{\lambda'}a_\lambda = 0} \text{ if } \lambda \neq \lambda' \qquad (5)$$

holds for all basis kets!

Summary: $\boxed{[a^\dagger_\lambda, a^\dagger_{\lambda'}]_\zeta = 0, \quad [a_\lambda, a_{\lambda'}]_\zeta = 0, \quad [a_\lambda, a^\dagger_{\lambda'}]_\zeta = \delta_{\lambda\lambda'}}$ (6)

'boson operators commute, fermion creation anti-commute', except for $[a_\lambda, a^\dagger_\lambda]_\zeta = 1$ (7)

Given complex structure of Fock space, these relations are remarkably simple!

Change of basis

The single-particle states used above must form a basis of $\mathcal{H}_{(1)}$, satisfying

	for discrete index		for continuous index, e.g. $\lambda = x$	
- orthogonality:	$\langle \lambda' \vert \lambda \rangle = \delta_{\lambda'\lambda}$	(1a)	$\langle x' \vert x \rangle = \delta(x'-x)$	(1b)
- completeness:	$\sum_\lambda \vert\lambda\rangle\langle\lambda\vert = \mathbb{1}$	(2a)	$\int dx\, \vert x\rangle\langle x\vert = \mathbb{1}$	(2b)
We make identifcation:	$\vert\lambda\rangle = a^\dagger_\lambda \vert\Omega\rangle$	(3a)	$\vert x\rangle = a^\dagger(x)\vert\Omega\rangle$	(3b)
Consider change of basis:	$\vert\tilde\lambda\rangle = \sum_\lambda \vert\lambda\rangle\langle\lambda\vert\tilde\lambda\rangle$	(4a)	$\vert p\rangle = \int dx\, \vert x\rangle\langle x\vert p\rangle$	(4b)
Correspondingly:	$a^\dagger_{\tilde\lambda} = \sum_\lambda a^\dagger_\lambda \langle\lambda\vert\tilde\lambda\rangle$	(5a)	$a^\dagger(p) = \int dx\, a^\dagger(x)\langle x\vert p\rangle$	(5b)
	$a_{\tilde\lambda} = \sum_\lambda \langle\tilde\lambda\vert\lambda\rangle a_\lambda$	(6a)	$a(p) = \int dx\, \langle p\vert x\rangle a(x)$	(6b)

(anti)-commutation relations preserve their form:

If $[a_\lambda, a^\dagger_{\lambda'}]_\zeta = \delta_{\lambda\lambda'}$, then (7a)

$$[a_{\tilde\lambda}, a^\dagger_{\tilde\lambda'}]_\zeta = \langle\tilde\lambda\vert\Big[\sum_{\lambda\lambda'} \vert\lambda\rangle \overbrace{[a_\lambda, a^\dagger_{\lambda'}]}^{(7a)\,\delta_{\lambda\lambda'}} \langle\lambda'\vert\Big]\vert\tilde\lambda'\rangle \qquad (8a)$$

$$= \langle\tilde\lambda\vert\sum_\lambda\vert\lambda\rangle\langle\lambda\vert\tilde\lambda'\rangle \overset{(2a)}{=} \langle\tilde\lambda\vert\,\mathbb{1}\,\vert\tilde\lambda'\rangle = \delta_{\tilde\lambda\tilde\lambda'} \qquad (9a)$$

If $[a_x, a^\dagger_{x'}]_\zeta = \delta(x-x')$, (7b)

then similarly,

$$[a_p, a^\dagger_{p'}]_\zeta = \delta(p-p') \qquad (9b)$$

Representation of one-body operators

Def: 'occupation number operator': $\hat n_\lambda = a^\dagger_\lambda a_\lambda$ with $\underset{\text{operator}}{\hat n_\lambda}\vert\ldots,n_\lambda,\ldots\rangle \overset{(11.2)}{=} \underset{\text{eigenvalue}}{n_\lambda}\vert\ldots,n_\lambda,\ldots\rangle$ (1)

Diagonal one-body operator: $\hat O_{(1)} = \sum_\lambda \vert\lambda\rangle O_\lambda \langle\lambda\vert$, $\quad O_{\lambda\lambda'} = \langle\lambda\vert\hat O\vert\lambda'\rangle = O_\lambda\delta_{\lambda\lambda'}$ (2)

When acting in $\mathcal{F}$: $\hat O = \sum_{N=0}^{\infty}\sum_{i=1}^{N} \mathbb{1}_{(1)} \oplus \ldots \oplus \mathbb{1}_{(1)} \oplus \hat O_{(1)} \oplus \mathbb{1}_{(1)} \oplus \ldots \oplus \mathbb{1}_{(1)}$ (3)

acts in i-th of N single-particle spaces: is the single particle there found in the single-particle state $\vert\lambda\rangle$?

Many-body matrix elements: total number of particles found in single-particle state λ

$$\langle n_0,n_1,n_2,\ldots\vert\,\hat O\,\vert n'_0,n'_1,n'_2,\ldots\rangle = \sum_\lambda \langle n_0,n_1,n_2,\ldots\vert\, O_\lambda n'_\lambda\,\vert n'_0,n'_1,n'_2,\ldots\rangle \qquad (4)$$

$$= \langle n_0,n_1,n_2,\ldots\vert\,\sum_\lambda O_\lambda \hat n_\lambda\,\vert n'_0,n'_1,n'_2,\ldots\rangle \qquad (5)$$

(5) holds for all basis kets of $\mathcal{F}$,

$\Rightarrow$ operator identity: $\boxed{\hat O = \sum_\lambda O_\lambda \hat n_\lambda} = \sum_\lambda a^\dagger_\lambda\langle\lambda\vert O\vert\lambda\rangle a_\lambda$ (6)

Simply count the number of particles in single-particle state λ and multiply by eigenvalue!

Transformed to a general (non-diagonal) basis: $\hat O = \sum_{\lambda\lambda'} a^\dagger_\lambda\langle\lambda\vert O\vert\lambda'\rangle a_{\lambda'} = \sum_{\lambda\lambda'} a^\dagger_\lambda O_{\lambda\lambda'} a_{\lambda'}$ (7)

Examples of one-body operators

Various single-particle bases: energy eigenbasis position basis momentum basis

Total particle number: $$\hat N = \sum_\lambda \hat n_\lambda = \int dx\, \underbrace{a^\dagger(x)\, a(x)}_{=\hat\rho(x)} = \int dp\, a^\dagger(p)\, a(p) \qquad (1)$$

$= \hat\rho(x)$ = density operator

Kinetic energy: $$\hat H_{kin} = \sum_\lambda \varepsilon_\lambda \hat n_\lambda = \int dp\, \frac{p^2}{2m}\, a^\dagger(p)\, a(p) \qquad (2)$$

Potential $$\hat H_{pot} = \int dx\, V(x)\, a^\dagger(x)\, a(x) \qquad (3)$$

Lattice Hamiltonian: $$\hat H_{lat} = \underbrace{\sum_i \varepsilon_i c^\dagger_i c_i}_{\text{on-site energy}} + \underbrace{\sum_{ij} t\,(c^\dagger_i c_j + c^\dagger_j c_i)}_{\text{hopping between sites i and j}} \qquad (4)$$

Zeeman field coupling to electron spin: $(\hbar = 1,\ g\mu_B = 1)$

$$\hat H_{Zeeman} = \sum_i \hat{\vec S}_i \cdot \vec B \qquad \hat{\vec S}_i = \sum_{\sigma\sigma'} a^\dagger_{i\sigma}\left(\tfrac12 \vec\tau_{\sigma\sigma'}\right) a_{i\sigma} \qquad (5)$$

spin operator Pauli matrices

$\sigma \in \uparrow, \downarrow$

Representation of two-body operators

Interaction potential between particles at positions x_i, x_j : $$\underbrace{V(x_i, x_j) = V(x_j, x_i)}_{\text{symmetric}} \qquad (1)$$

We seek many-body operator $\hat V$ such that

$$\hat V\, |x_1, x_2, \dots, x_N\rangle = \sum_{i<j}^{N} V(x_i, x_j)\, |x_1, x_2, \dots, x_N\rangle = \frac12 \sum_{i \neq j}^{N} V(x_i, x_j)\, |x_1, x_2, \dots, x_N\rangle \qquad (2)$$

Ansatz: $$\boxed{\hat V = \frac12 \int dx \int dx'\; a^\dagger(x)\, a^\dagger(x')\; V(x, x')\; a(x')\, a(x)} \qquad (3)$$

Interpretation: 'take out two particles at x and x', let them feel the interaction, and put them back in'.

Note: $$a(x)\, a^\dagger(x_i) \overset{(13.7b)}{=} \zeta\, a^\dagger(x_i)\, a(x) + \delta(x - x_i) \qquad (4)$$

Check (3): act with $\hat V$ on N-particle position eigenstate:

$$a^\dagger(x) a^\dagger(x') a(x') a(x)\, |x_1, x_2, \dots, x_i, \dots, x_N\rangle = a^\dagger(x) a^\dagger(x') a(x')\, a(x)\, a^\dagger(x_1)\, a^\dagger(x_2) \dots a^\dagger(x_i) \dots a^\dagger(x_N)\, |\Omega\rangle \qquad (5)$$

commute $a(x)$ to the right: vacuum state is empty: $a(x)|\Omega\rangle = 0$

each commutation operation yields an extra $\delta(x - x_i)$

$$\overset{(4)}{=} \sum_{i=1}^{N} \delta(x - x_i)\, \zeta^{i-1}\; a^\dagger(x) \underbrace{a^\dagger(x') a(x')}_{\hat\rho(x')}\; a^\dagger(x_1) \dots a^\dagger(x_{i-1})\, a^\dagger(x_{i+1}) \dots a^\dagger(x_N)\, |\Omega\rangle \qquad (6)$$

density operator 'finds' the particles, yields $\sum_{j \neq i}^{N} \delta(x' - x_j)$

commute $a^\dagger(x)$ to the right until it sits between $a^\dagger(x_{i-1})$, $a^\dagger(x_{i+1})$

$$\overset{(5)}{=} \sum_{i=1}^{N} \delta(x-x_i) \sum_{j\neq i}^{N} \delta(x'-x_j) \underbrace{\varsigma^{i-1}\,\varsigma^{i-1}}_{=1}\; a^\dagger(x_1) \dots a^\dagger(x_{i-1})\, \underbrace{a^\dagger(x)}_{=x_i}\, a^\dagger(x_{i+1}) \dots a^\dagger(x_N)|\Omega\rangle \qquad (1)$$

Now multiply by $\frac{1}{2}V(x,x')$ and integrate over x and x', as in (16.3): (2)

$$\hat{V}\,|x_1,x_2,\dots,x_N\rangle = \frac{1}{2}\int dx \int dx' \,\frac{1}{2}V(x,x')\, \underbrace{a^\dagger(x)a^\dagger(x')a(x')a(x)\,|x_1,x_2,\dots,x_i,\dots,x_N\rangle}_{=(17.1)} \qquad (3)$$

$$\overset{(1)}{=} \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N} V(x_i,x_j)\, \underbrace{a^\dagger(x_1)\dots a^\dagger(x_{i-1})\,a^\dagger(x_i)\,a^\dagger(x_{i+1})\dots a^\dagger(x_N)|\Omega\rangle}_{=|x_1,x_2,\dots,x_N\rangle} \qquad (4)$$

$$= (16.2) \;\checkmark$$

Hence, Ansatz (16.3) does yield the result (16.2), as required.

A general two-body operator with matrix elements $\langle\lambda,\eta|\hat{O}|\lambda',\eta'\rangle$ can be expressed as

$$\boxed{\hat{O} = \sum_{\lambda\eta,\lambda'\eta'} a^\dagger_\lambda\, a^\dagger_\eta\, \langle\lambda,\eta|\hat{O}|\lambda',\eta'\rangle\, a_{\eta'}\, a_{\lambda'}} \qquad (5)$$

mnemonic: $|\lambda,\eta\rangle\langle\lambda,\eta|\hat{O}|\lambda',\eta'\rangle\langle\lambda',\eta'|$