Second Quantization

Note Title 10/29/2009

Altland & Simons (2006)
Chap. 2 (p. 39ff)

Lecture notes
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Motivation

- theoretical cornerstone of quantum field theories → quantum many body physics
  Q: $\langle \hat{c}(\vec{r}_2, t_2) \hat{c}^\dagger(\vec{r}_1, t_1) \rangle = ?$
- "2nd quantization"
  - quantization of whether or not particle is in a certain state
  → creation / annihilation operators of particles in a specific state

Ex, single particle Hamiltonian

$$\hat{H} |n\rangle = E_n |n\rangle \qquad \text{with} \quad \langle \vec{r} | n \rangle =: \psi_n(\vec{r}) \tag{1}$$

e.g. free particles $\hat{H}^{(N)} = \sum_i^N \frac{\hat{p}_i^2}{2m}$

symmetric under particle exchange ! (2)

$$\Rightarrow \quad P_{12}^2 \, \psi(\vec{r}_1, \vec{r}_2) = +1 \cdot \psi(\vec{r}_1, \vec{r}_2) \tag{3}$$

↳ eigenvalues under particle exchange

-1 : Fermions $\psi_F = \frac{1}{\sqrt{2}} \left(\langle \vec{r}_1 | 1 \rangle \langle \vec{r}_2 | 2 \rangle - \langle \vec{r}_1 | 2 \rangle \langle \vec{r}_2 | 1 \rangle \right)$

$+1$: Bosons $\psi_B = \frac{1}{\sqrt{2}} \left(\text{—} \; \text{''} \; \text{—} \; + \; \text{—} \; \text{''} \; \text{—} \right)$

more generally (Fermions): Slater determinant

$$\Psi_{1\ldots N}(\vec{r}_1, \ldots, \vec{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \langle \vec{r}_1 | 1 \rangle & \langle \vec{r}_1 | 2 \rangle & \cdots & \langle \vec{r}_1 | N \rangle \\ \langle \vec{r}_2 | 1 \rangle & \langle r_2 | 2 \rangle & & \vdots \\ \vdots & & \ddots & \vdots \\ \langle \vec{r}_N | 1 \rangle & \cdots & & \langle \vec{r}_N | N \rangle \end{vmatrix} \qquad (4)$$

particle must be in different states (otherwise $\psi = 0$)

for consistency $\Rightarrow$ Pauli exclusion principle

- decide on order of columns ("state order")
- decide on order of rows (e.g. in 1D: $r_1 < r_2 < \ldots < r_N$)

$\Rightarrow$ sufficient to write

$$|\psi\rangle = |1, 2, \ldots, N\rangle \qquad (5)$$

e.g. for two particles

$|\psi\rangle = |1, 2\rangle$ one particle in state 1, the other in state 2

or $|1, 5\rangle$ 1 5

or $|2, 4\rangle$ 2 4

... ...

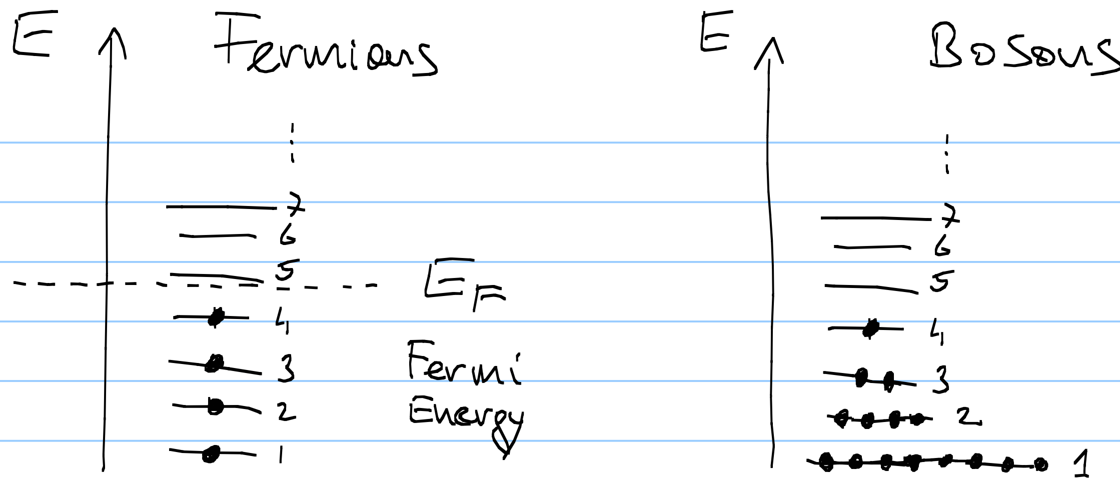
or equivalently, in terms of "creation" operators $c_i^\dagger$

$|\psi\rangle = c_1^\dagger c_2^\dagger |\,\rangle$ with $|\,\rangle$ being the empty state with no particles.

or $c_1^\dagger c_5^\dagger |\,\rangle$

or $c_2^\dagger c_4^\dagger |\,\rangle$

...



(6)

$|\psi\rangle_F = |1234\rangle$

$\langle n_i \rangle \leq 1 \Rightarrow$ Fermi sea

$|\psi\rangle_B = |11111111\,2222\,334\rangle$

$\hookrightarrow$ all particles can condensate in lowest single particle level!

Occupation number representation (Fock space)

$$|\psi_F\rangle = |\underline{1}\ \underline{1}\ \underline{1}\ \underline{1}\ \underline{0}\ \underline{0}\ \underline{0}\ \underline{0} \dots \rangle$$

$$|\psi_B\rangle = |\underline{8}\ \underline{4}\ \underline{2}\ \underline{1}\ \underline{0}\ \underline{0}\ \underline{0}\ \underline{0} \dots \rangle \tag{7}$$

Hilbert space

$$\hat H^{(N)} = \sum_{i=1}^{N} \hat H_i = \hat H^{(1)} \otimes 1 \otimes \dots \otimes 1 + 1 \otimes \hat H^{(1)} \otimes \dots \otimes 1 + \dots + 1 \otimes 1 \otimes \dots \hat H^{(1)} \tag{8}$$

- state space dimension exponentially enlarged!
- in general many body state can be arbitrarily complex

$$|\psi\rangle = \sum_{n_1, n_2, \dots} C_{n_1, n_2, \dots} |n_1 n_2 \dots\rangle \tag{9}$$

"many Slater determinants"

Creation annihilation operators

recall: harmonic oscillator

$$\hat{a}^{\dagger}|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{10}$$

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

such that $\underbrace{\hat{a}^{\dagger}\hat{a}}_{\equiv \hat{n}}|n\rangle = (\sqrt{n})^2|n\rangle = n|n\rangle$ (11)

<u>generalize</u>: define linear map

<u>Def</u> $a_i^{\dagger}\,|n_1, n_2, \ldots, n_i, \ldots\rangle = \sqrt{n_i+1}\; S_i\, |n_1, n_2, \ldots, n_i+1, \ldots\rangle$

possible sign

where $S_i \equiv \zeta^{q_i}$ with $q_i \equiv \sum_{i'<i} n_{i'}$

and $\zeta \equiv +1$ for bosons (12)

-1 for fermions

<u>claim</u> $[a_i^{\dagger}, a_j^{\dagger}]_{\zeta} = 0$ (13)

where $[\hat{A}, \hat{B}]_{\zeta} \equiv \hat{A}\hat{B} - \zeta\hat{B}\hat{A}$ (14)

e.g. commutator $[A,B] = [A,B]_{-1}$

anti-commutator $\{A,B\} = [A,B]_{+1}$

proof, for $i=j$: bosons $[a^\dagger, a^\dagger] = a^\dagger a^\dagger - a^\dagger a^\dagger = 0$ ✓

fermions $\{a^\dagger, a^\dagger\} = 0$ since $(a_i^\dagger)^2 = 0$

for $i \neq j$ it is sufficient to show

$$\underbrace{\left(a_i^\dagger a_j^\dagger - \zeta\, a_j^\dagger a_i^\dagger\right)}_{=0} |n_1, n_2, \dots\rangle = 0 \quad \text{for all states!}$$

assuming $i<j$ without restricting the case

$$a_i^\dagger a_j^\dagger |n_1 n_2, \dots, \underbrace{n_i}_{\downarrow\, n_i+1} \dots \underbrace{n_j}_{\downarrow\, n_j+1} \dots\rangle$$

$$(\pm 1)^{2\sum_{i'<i} n_{i'}} = +1$$

(sign if any cancels!)

$$= \sqrt{n_i+1}\sqrt{n_j+1} \cdot S \cdot |n_1, n_2, \dots, n_i+1, \dots, n_j+1, \dots\rangle$$

where $S = \zeta^{\left(n_i + \sum_{k=i+1}^{j} n_k\right)}$

similarly

$$\hat{a}_j^\dagger \hat{a}_i^\dagger |n_1, n_2, \dots \underbrace{n_i}_{\downarrow\, n_i+1} \dots \underbrace{n_j}_{\downarrow\, n_j+1} \dots\rangle$$

$$= \sqrt{n_i+1}\sqrt{n_j+1} \cdot S \cdot |n_1, n_2, \dots, n_i+1, \dots, n_j+1, \dots\rangle$$

where $S = \zeta^{\left(n_i + 1 + \sum_{k=i+1}^{j} n_k\right)}$

$$\Rightarrow \quad \underbrace{a_i^\dagger a_j^\dagger = \zeta \cdot a_j^\dagger a_i^\dagger}$$

since $(\pm 1)^2 = 1$

q. e. d.

from the definition of $a_i^\dagger$ in (12)

$$\langle n_1', n_2', \dots, n_i', \dots | \hat{a}_i | n_1, n_2, \dots, n_i, \dots \rangle$$

$$= \langle n_1, n_2, \dots, n_i, \dots | \hat{a}_i^\dagger | n_1', n_2', \dots, n_i', \dots \rangle^*$$

$$= \underbrace{s_i'}_{=s_i} \underbrace{\sqrt{n_i'+1}}_{=n_i} \delta_{n_1, n_1'} \delta_{n_2 n_2'} \cdots \delta_{n_i, n_i'+1} \cdots$$

$$\Rightarrow \hat{a}_i | n_1, n_2, \dots n_i, \dots \rangle = \sqrt{n_i}\, s_i | n_1, n_2, \dots, n_i - 1, \dots \rangle$$

"annihilation operator" (15)

with $s_i \equiv (\pm 1)^{\sum_{i'<i} n_{i'}}$ (same as in (12))

$$\Rightarrow (13) \quad [\hat{a}_i, \hat{a}_j]_\xi = \left([\hat{a}_j^\dagger, \hat{a}_i^\dagger] \right)^\dagger = 0 \qquad (16)$$

Similarly: [EXERCISE]

$$[\hat{a}_i, \hat{a}_j^\dagger]_\xi = \delta_{ij} \qquad (17)$$

NB! creation/annihilation operator algebra completely (18) defined by the canonical commutator relations (CCR) given in (13), (16), and (17), together with the existence of the empty state $|\rangle$ defined by

$$\forall_i \; \hat{a}_i^\dagger | \rangle = 0 \qquad (19)$$

NB! CCR are invariant under change of local basis (20)
$|i\rangle \longrightarrow |\tilde{k}\rangle = \sum_i u_{ik} |i\rangle \Rightarrow \tilde{a}_k = \sum_i u_{ik} \hat{a}_k$ [EXERCISE]

e.g. bosons: $[a, a^\dagger] = 1$

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

$$\Rightarrow \hat{N} (a^\dagger)^n |\rangle = a^\dagger a \cdot \underbrace{a^\dagger \cdots a^\dagger}_{n \text{ times}} |\rangle$$

$$= a^\dagger \cdot a \cdot a^\dagger a^\dagger \cdot \ldots \cdot a^\dagger |\rangle$$

$$a a^\dagger = a^\dagger a + 1$$

$$= n \cdot (\hat{a}^\dagger)^n |\rangle + \cancel{(a^\dagger)^n \underbrace{a |\rangle}_{=0}}$$

$\Rightarrow (\hat{a}^\dagger)^n |\rangle$ is (unnormalized) eigenvector of $\hat{N}$

$$|n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n |\rangle$$

with the normalization determined as follows

$$\langle | (\hat{a})^n (\hat{a}^\dagger)^n | \rangle = \langle | \underbrace{a \cdot a \cdots a}_{n\text{-times}} \underbrace{a^\dagger \cdots a^\dagger a^\dagger}_{n\text{-times}} | \rangle$$

$$= n \cdot \langle | \underbrace{a \cdot a \cdots a}_{(n-1) \text{ times}} \underbrace{a^\dagger a^\dagger \cdots}_{(n-1) \text{ times}} | \rangle + \cancel{\langle | \underbrace{a \cdot a \cdots a^\dagger}_{(n-1)\times} \underbrace{\cdots a^\dagger}_{n\times} \underbrace{\cdot a |\rangle}_{=0}}$$

...

$$= n(n-1)(n-2) \cdot \ldots \cdot 1 \cdot \underbrace{\langle | \rangle}_{=1} = n!$$

NB! empty state is a properly normalized state!

specifically: $$a^\dagger |n\rangle = \sqrt{n+1} \underbrace{\frac{1}{\sqrt{(n+1)!}} (a^\dagger)^{n+1} |\rangle}_{= |n+1\rangle}$$

Independence of canonical commutator relations (CCR) under rotation of single particle basis

complete basis $|i\rangle \equiv \hat{a}_i^{+}|\rangle$

$\hookrightarrow \quad \sum_i |i\rangle\langle i| = \hat{\mathbb{1}}$

unitary transformation U : $|\tilde{k}\rangle = \sum_i u_{ik} |i\rangle$

$\hookrightarrow \quad \tilde{a}_k = \sum_i u_{ik} \hat{a}_i$

$$\Rightarrow \left[\tilde{a}_k, \tilde{a}^{+}_{k'}\right]_{\xi} = \sum_{ii'} u_{ik} u^{*}_{i'k'} \underbrace{\left[a_i, \hat{a}^{+}_{i'}\right]_{\xi}}_{\underset{(17)}{=} \delta_{ii'}}$$

$$= \sum_i u_{ik} u^{*}_{ik'} = \delta_{kk'}$$

$\Rightarrow$ $\hat{a}_k$ <u>obey</u> the same CCR!

Commutator Algebra

- $\zeta [A,B]_\zeta = \zeta (AB - \zeta BA) = -(BA - \zeta AB)$ $\quad$ (20)

$\qquad = -[B,A]_\zeta$ $\quad (\zeta = \pm 1)$

- $[\hat{A}_1 \hat{A}_2 \dots \hat{A}_m, \hat{B}_1 \dots \hat{B}_n]_{\cancel{\zeta}} =$

plain commutator with at least m or n even

$= \sum$ all possible pairwise commutators $[\hat{A}_i, \hat{B}_j]_\zeta$
× "ordered" product of remaining operators
× possibly a minus sign $\quad$ (21)

("Wicks theorem")

$\underline{\text{Ex}}$ $\quad [A_1 \cdot A_2, B] = A_1 [A_2, B]_\zeta + \zeta [A_1, B] \cdot A_2$

since $\quad$ (22)

$$A_1 A_2 \cdot B = A_1 \left([A_2, B]_\zeta + \zeta B A_2 \right)$$

$$= A_1 [A_2, B] + \zeta A_1 B A_2$$

$$= A_1 [A_2, B] + \zeta [A_1, B] A_2 + \underbrace{\zeta^2}_{=+1} B A_1 A_2$$

e.g. $[\hat{a}_i^\dagger \hat{a}_j, a_k^\dagger] = \underline{a_i^\dagger \delta_{jk}}$

Operator Representation

<u>occupation number operator</u>

$$\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i \tag{23}$$

$$\Rightarrow \hat{n}_i \, |n_1, n_2, \ldots n_i, \ldots \rangle = \left(\sqrt{n_i}\right)^2 |n_1, n_2, \ldots n_i \ldots \rangle$$

$$= n_i \, |n_1, n_2, \ldots n_i, \ldots \rangle$$

total number of particles $\hat{N} = \sum_i \hat{a}_i^\dagger \hat{a}_i$ (24)

$$\hat{N} \, |n_1, n_2, \ldots \rangle = \left(\sum_i n_i\right) |n_1, n_2, \ldots \rangle$$

<u>one body operator</u>

first, assume operator is diagonal in number operator basis

$$\hat{O}_1 = \sum_i h_i \, |i\rangle\langle i| \equiv \sum_i h_i \, \hat{a}_i^\dagger \hat{a}_i$$

$\big\downarrow$ rotate to arbitrary 1-particle basis

$$\hat{O}_1 = \sum_{ij} h_{ij} \, a_i^\dagger a_j$$

… general form of 1-particle operator in 2nd quantization

with $h_{ij} \equiv \langle i | O_1 | j \rangle$

(25)

Ex) Spin operator

$$\vec{S} = \sum_{i} \hat{a}^{\dagger}_{i\sigma} \, \vec{S}_{\sigma\sigma'} \, \hat{a}_{i'\sigma'} \qquad (26)$$

with $S_\alpha = \frac{1}{2}\sigma_\alpha \quad (\alpha = x, y, z)$

and Pauli matrizes $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

(27)

[EXERCISE]
check spin commutator rel.

Ex) 1-particle Hamiltonian

$$H = \int d^3\vec{r} \; a^{\dagger}(\vec{r}) \left(\frac{\vec{p}^{\,2}}{2m} + V(\vec{r}) \right) \hat{a}(r)$$

$$\left(\vec{p} = \frac{\hbar}{i} \vec{\nabla} \right) \qquad (28)$$

Ex) local density operator

$$\hat{\rho}(r) = \hat{a}^{\dagger}(r) \, \hat{a}(r) \qquad (29)$$

2-body operator (interaction)

expect

$$\hat{V}|\vec{r}_1,\vec{r}_2,\dots\rangle = \frac{1}{2}\sum_{i\neq j} V(\vec{r}_i,\vec{r}_j)\,|\vec{r}_1,\vec{r}_2,\dots\rangle$$

$$= \sum_{i<j} V(\vec{r}_i,\vec{r}_j)\,|\vec{r}_1,\vec{r}_2,\dots\rangle \qquad (30)$$

having $\quad [\hat{a}(\vec{r}),\hat{a}^+(\vec{r}\,')] = \delta(\vec{r}-\vec{r}\,') \qquad (31)$

discrete → continuum transition

$$\Rightarrow [\hat{a}^+(\vec{r})\underbrace{\hat{a}(\vec{r}),\hat{a}^+(\vec{r}\,')}_{(22)}] = \delta(\vec{r}-\vec{r}\,')\cdot a^+(\vec{r}) \qquad (32)$$

claim,

$$\hat{V} = \frac{1}{2}\int d^3\vec{r}\int d^3\vec{r}\,'\ \hat{a}^+(\vec{r})\,\hat{a}^+(\vec{r}\,')\cdot V(\vec{r},\vec{r}\,')\cdot\hat{a}(\vec{r}\,')\,\hat{a}(\vec{r}) \qquad (33)$$

— note the order in $\hat{a}$ operators!
e.g. reversed order of the a^+a^+ compared to the aa term (w.r.t. $\vec{r}$ and $\vec{r}\,'$)

(NB! also required so $\hat{V}$ is hermitian!)

proof:

taking first the operator part of (33)

$$\hat{a}^\dagger(\vec{r})\,\hat{a}^\dagger(\vec{r}')\,\hat{a}(\vec{r}')\,\hat{a}(\vec{r})\,|\vec{r}_1 \dots \vec{r}_N)$$

$$= \hat{a}^\dagger(\vec{r})\,\underbrace{\hat{a}^\dagger(\vec{r}')\,\hat{a}(\vec{r}')}_{=\hat{\rho}(\vec{r}')}\,\hat{a}(\vec{r})\cdot\hat{a}^\dagger(\vec{r}_1)\cdots\hat{a}^\dagger(\vec{r}_N)\,|\,\rangle$$

$$\overset{(31),(32)}{=} \sum_{i=1}^{N} \xi^{i-1}\,\delta(\vec{r}-\vec{r}_i)\sum_{j\neq i}^{N}\delta(\vec{r}'-\vec{r}_j)\;*$$

$$*\;\hat{a}^\dagger(\vec{r}_i)\cdot\hat{a}^\dagger(\vec{r}_1)\cdots\hat{a}^\dagger(\vec{r}_{i-1})\cdot\hat{a}^\dagger(\vec{r}_{i+1})\cdots\hat{a}^\dagger(\vec{r}_N)$$

→ another sign factor ξ^{i-1}

↳ cancels the existing ξ^{i-1}

$$= \sum_{i\neq j}^{N} \delta(\vec{r}-\vec{r}_i)\,\delta(\vec{r}'-\vec{r}_j)\,|\vec{r}_1,\vec{r}_2,\dots,\vec{r}_N)$$

now adding the remainder of (33)

$$\hat{V}\,|\vec{r}_1,\vec{r}_2,\dots,\vec{r}_N) =$$

$$= \frac{1}{2}\int d^3\vec{r}\int d^3\vec{r}'\,V(\vec{r},\vec{r}')\;*\sum_{i\neq j}\delta(\vec{r}-\vec{r}_i)\,\delta(\vec{r}'-\vec{r}_j)\,|\vec{r}_1,\dots\vec{r}_N)$$

$$= \left(\frac{1}{2}\sum_{i\neq j} V(\vec{r}_i,\vec{r}_j)\right)|\vec{r}_1,\dots,\vec{r}_N)$$

q.e.d.