Quantum many-body theory basics

Three assumptions to construct the quantum theory of many particles:

1. Single-particle wave function extends to N-particle wave function.

$$\psi(\vec{r}) \in \mathbb{C} \qquad \psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N) \in \mathbb{C}$$

$|\psi(\vec{r}_1, \cdots, \vec{r}_N)|^2 \prod_{j=1}^{N} d\vec{r}_j$ = probability for finding particles within the infinitesimal volume surrounding $(\vec{r}_1, \cdots, \vec{r}_N)$

2. Identical particles having e.g. same mass, charge, and spin are indistinguishable.

$$P_{jk}\psi(\cdots, \vec{r}_j, \cdots, \vec{r}_k, \cdots) = \lambda\psi(\cdots, \vec{r}_k, \cdots, \vec{r}_j, \cdots)$$ (identical up to sign)

$$P_{jk}^2\psi = \psi \rightarrow \lambda^2 = 1 \rightarrow \lambda = +1$$ (boson), -1 (fermion)

Note: In 2d, there are quasiparticles that give arbitrary $\lambda = e^{i\theta}$ or even don't satisfy the identity. These are called anyons.

3. Single- and few-particle operators remain unchanged when acting on N-particle states.

Many-body states in first quantization

Single-particle basis: $|\nu\rangle$ (spin, orbital, momentum, etc.)

$\psi_\nu(\vec{r}) = \langle \vec{r}|\nu\rangle$

Ex) free electrons: $\nu = (\vec{k}, \sigma)$ electrons in an atom: $\nu = (n, l, m, \sigma)$

$\int d\vec{r}\, |\vec{r}\rangle\langle\vec{r}| = 1$

Orthonormality: $\langle \nu|\nu'\rangle = \delta_{\nu\nu'}$ Completeness: $\sum_\nu |\nu\rangle\langle\nu| = 1$

$\langle \vec{r}|\vec{r}'\rangle = \delta(\vec{r}-\vec{r}')$

1st assumption

2nd: (anti-)symmetrization

$$\underbrace{S_{\pm}}_{\text{2nd}}\ \overbrace{\prod_{j=1}^{N} \langle \vec{r}_j|\nu_j\rangle}^{\text{1st assumption}} \propto \begin{vmatrix} \langle \vec{r}_1|\nu_1\rangle & \langle \vec{r}_1|\nu_2\rangle & \cdots & \langle \vec{r}_1|\nu_N\rangle \\ \langle \vec{r}_2|\nu_1\rangle & \langle \vec{r}_2|\nu_2\rangle & \cdots & \langle \vec{r}_2|\nu_N\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \vec{r}_N|\nu_1\rangle & \langle \vec{r}_N|\nu_2\rangle & \cdots & \langle \vec{r}_N|\nu_N\rangle \end{vmatrix}_{\pm}$$

Boson:
permanent

$$|\cdot\cdot|_+ = \sum_{p\in S_N} \left(\prod_{j=1}^{N} \langle \vec{r}_j|\nu_{p(j)}\rangle \right)$$

Group of $N!$ permutations

$(1, 2, \cdots, N) \to (p(1), p(2), \cdots, p(N))$

Fermion:
Slater determinant

$$|\cdot\cdot|_- = \sum_{p\in S_N} \left(\prod_{j=1}^{N} \langle \vec{r}_j|\nu_{p(j)}\rangle \right) \mathrm{sgn}(p)$$

$= (-1)^{\#\text{ of exchanging neighbors permuting } (1\,2\cdots N) \text{ to } (p(1)\cdots p(N))}$

Ex) $\mathrm{sgn}(1\,2\,3) = 1$

$\mathrm{sgn}(2\,1\,3) = -1$

$\mathrm{sgn}(2\,3\,1) = -1$

Check: $\nu_j = \nu_k$ leads to $|\cdot\cdot|_- = 0$

Operators in first quantization

$$\int d\vec{r}\, |\vec{r}\rangle\langle\vec{r}| = \sum_{\nu} |\nu\rangle\langle\nu| = 1$$

One-particle operators: $T_{tot} = \sum_{j=1}^{N} T_j$ (3rd assumption)

$$T_j = T(\vec{r}, \vec{\nabla}) = \int d\vec{r}\, |\vec{r}\rangle T(\vec{r}, \vec{\nabla}) \langle\vec{r}| = \sum_{\nu_j'} \sum_{\nu_j} |\nu_j'\rangle \underbrace{\int d\vec{r} \langle\nu_j'|\vec{r}\rangle T(\vec{r}, \vec{\nabla}) \langle\vec{r}|\nu_j\rangle}_{= T_{\nu_j'\nu_j}} \langle\nu_j|$$

external potential kinetic energy

Two-particle operators: $V_{tot} = \frac{1}{2} \sum_{j \neq k} V_{jk}$

Coulomb interaction

$$V_{jk} = \sum_{\nu_j'} \sum_{\nu_k'} \sum_{\nu_j} \sum_{\nu_k} |\nu_j'\rangle |\nu_k'\rangle \underbrace{\int d\vec{r}\, d\vec{r}\,' \langle\nu_k'|\vec{r}\,'\rangle \langle\nu_j'|\vec{r}\rangle V(\vec{r} - \vec{r}\,') \langle\vec{r}|\nu_j\rangle \langle\vec{r}\,'|\nu_k\rangle}_{= V_{\nu_j'\nu_k'\nu_j\nu_k}} \langle\nu_k| \langle\nu_j|$$

Q: Can one make a more compact notation?

Second quantization

Occupation number representation: $|n_{\nu_1}, n_{\nu_2}, n_{\nu_3}, \cdots\rangle$

$\nu_1, \nu_2, \nu_3, \cdots$

→ order matters!

particles occupying the ν_j-basis:

$$n_{\nu_j} = \begin{cases} 0,\ 1 & \text{(fermion)} \\ 0,\ 1,\ 2,\ 3,\ \cdots & \text{(boson)} \end{cases}$$

< Bosons >

Define the annihilation operator: $b_{\nu_j}|n_{\nu_j}\rangle = \begin{cases} B(n_{\nu_j})|n_{\nu_j}-1\rangle & \text{if } n_{\nu_j} > 0 \\ 0 & \text{if } n_{\nu_j} = 0 \end{cases}$ $\quad B(n_{\nu_j}) \in \mathbb{R}$ (phase can be absorbed)

Then the creation operator is given by the hermitian conjugate: $b^\dagger_{\nu_j}|n_{\nu_j}-1\rangle = B(n_{\nu_j})|n_{\nu_j}\rangle$

$$(\because \langle n'|b_{\nu_j}|n_{\nu_j}\rangle = B(n_{\nu_j})\delta_{n'+1,n_{\nu_j}} = \langle n_{\nu_j}|b^\dagger_{\nu_j}|n'\rangle^* \delta_{n',n_{\nu_j}-1})$$

$$\begin{tikzcd}
0 \arrow[r, bend left, "\times"] & {|0\rangle} \arrow[l, bend left, "b"] \arrow[r, bend left, "b^\dagger"] & {|1\rangle} \arrow[l, bend left, "b"] \arrow[r, bend left, "b^\dagger"] & {|2\rangle} \arrow[l, bend left, "b"] \arrow[r, bend left, "b^\dagger"] & {|3\rangle} \arrow[l, bend left, "b"] \arrow[r, bend left, "b^\dagger"] & \cdots \arrow[l, bend left, "b"]
\end{tikzcd}$$

Define the commutation relations:

$$[O_1, O_2] = [O_1, O_2]_- = O_1O_2 - O_2O_1$$

$$[O_1, O_2]_- = 0 \iff O_1O_2 = O_2O_1$$

$$[b_{\nu_j}, b_{\nu_k}] = [b^\dagger_{\nu_j}, b^\dagger_{\nu_k}] = 0, \quad [b_{\nu_j}, b^\dagger_{\nu_k}] = \delta_{\nu_j\nu_k}$$

Show: $b_\nu^\dagger b_\nu$ is the number operator that counts n_ν

① $b_\nu^\dagger b_\nu |\underbrace{n_\nu}_{\text{If } >0,\ =0}\rangle = \underbrace{\left(C(n_\nu)\right)^2}_{>0,\ =0} |n_\nu\rangle$

② $\underbrace{[b_\nu^\dagger b_\nu, b_\nu]}_{\downarrow} = b_\nu^\dagger b_\nu b_\nu - b_\nu b_\nu^\dagger b_\nu = [b_\nu^\dagger, b_\nu] b_\nu = -b_\nu$

$[(b_\nu^\dagger b_\nu) b_\nu - b_\nu (b_\nu^\dagger b_\nu)]|n_\nu\rangle = [(B(n_\nu-1))^3 B(n_\nu) - (B(n_\nu))^3]\,|n_\nu-1\rangle$

$= -B(n_\nu)|n_\nu-1\rangle$

$\Rightarrow (B(n_\nu))^2 - (B(n_\nu-1))^2 = 1 \Rightarrow (B(n_\nu))^2 = n_\nu$

③ $[b_\nu^\dagger b_\nu, b_\nu^\dagger] = b_\nu^\dagger$

$\therefore\ b_\nu^\dagger |n_\nu\rangle = \sqrt{n_\nu+1}\,|n_\nu+1\rangle$, $b_\nu|n_\nu\rangle = \sqrt{n_\nu}\,|n_\nu-1\rangle$,

$b_\nu^\dagger b_\nu |n_\nu\rangle = n_\nu |n_\nu\rangle$

Fock state: $|n_{\nu_1}, n_{\nu_2}, \cdots\rangle = \dfrac{1}{\sqrt{n_{\nu_1}!\, n_{\nu_2}! \cdots}} \underbrace{(b_{\nu_1}^\dagger)^{n_{\nu_1}} (b_{\nu_2}^\dagger)^{n_{\nu_2}} \cdots}_{\Downarrow} \underbrace{|0\rangle}_{\text{vacuum}}$

$$(\overbrace{b_{\nu_1}^\dagger\ b_{\nu_1}^\dagger \cdots}^{n_{\nu_1}})(\overbrace{b_{\nu_2}^\dagger\ b_{\nu_2}^\dagger \cdots}^{n_{\nu_2}})(\cdots)$$

order: 1 2 $\cdots$ $n_{\nu_1}+1$ $n_{\nu_1}+2$ $\cdots$

P_{jk}

Any exchange does not change the state

Fock states are automatically symmetrized!

< Fermions >

Define the annihilation operator: $c_{\nu_j}|n_{\nu_j}\rangle = \begin{cases} C(n_{\nu_j})\,|n_{\nu_j}-1\rangle & \text{if } n_{\nu_j}>0 \\ 0 & \text{if } n_{\nu_j}=0 \end{cases}$

Then the creation operator is given by the hermitian conjugate: $c^\dagger_{\nu_j}|n_{\nu_j}-1\rangle = C(n_{\nu_j})\,|n_{\nu_j}\rangle$

Define the commutation relations:

$$\{O_1,O_2\} = [O_1,O_2]_+ = O_1O_2+O_2O_1$$

$$\underline{\{c_{\nu_j},c_{\nu_k}\} = \{c^\dagger_{\nu_j},c^\dagger_{\nu_k}\} = 0,}\quad \{c_{\nu_j},c^\dagger_{\nu_k}\} = \delta_{\nu_j,\nu_k}$$

$$c_\nu^2 = 0,\quad (c^\dagger_\nu)^2 = 0$$

$$\begin{tikzcd} 0 \arrow[r, bend left, "\cancel{\ }"] & {|0\rangle} \arrow[l, bend left, "c"] \arrow[r, bend left, "c^\dagger"] & {|1\rangle} \arrow[l, bend left, "c"] \arrow[r, bend left, "c^\dagger"] & 0 \arrow[l, bend left, "\cancel{\ }"] \end{tikzcd}$$

$$[O_1,O_2]_+ = 0$$
$$\Updownarrow$$
$$O_1O_2 = -O_2O_1$$

① $c^\dagger_\nu c_\nu|n_\nu\rangle = (C(n_\nu))^2|n_\nu\rangle$

② $[c^\dagger_\nu c_\nu, c_\nu] = -c_\nu c^\dagger_\nu c_\nu = -c_\nu(1-c_\nu c^\dagger_\nu) = -c_\nu$

③ $[c^\dagger_\nu c_\nu, c^\dagger_\nu] = c^\dagger_\nu$

$\Rightarrow$

$c_\nu|n_\nu=1\rangle = |n_\nu=0\rangle$

$c^\dagger_\nu|n_\nu=0\rangle = |n_\nu=1\rangle$

$c^\dagger_\nu c_\nu|n_\nu\rangle = n_\nu|n_\nu\rangle$

Fock state: $|n_{\nu_1}, n_{\nu_2}, \cdots\rangle = (c^\dagger_{\nu_1})^{n_{\nu_1}} (c^\dagger_{\nu_2})^{n_{\nu_2}} \cdots |0\rangle$ $\qquad n_\nu = 0, 1$

$$\cdots c^\dagger_{\nu_j} \underbrace{(c^\dagger_{\nu_{j+1}})^{n_{\nu_{j+1}}} \cdots (c^\dagger_{\nu_{k-1}})^{n_{\nu_{k-1}}}}_{m = \sum_{i=j+1}^{k-1} n_{\nu_i} \text{ operators}} \nu_k \cdots$$

① gains a sign factor $(-1)^m$

② gains a sign factor $(-1)^{m+1}$

total: $(-1)^{2m+1} = -1$

Fock states are automatically anti-symmetrized!

Operators in second quantization

One-particle operators: $T_{tot} = \sum_{j=1}^{N} T_j \qquad T_j = \sum_{\nu_j'} \sum_{\nu_j} |\nu_j'\rangle \overbrace{\int d\vec{r} \langle \nu_j' | \vec{r}\rangle T(\vec{r}, \vec{\nabla}) \langle \vec{r} | \nu_j \rangle}^{= T_{\nu_j' \nu_j}} \langle \nu_j|$

Action of $|\nu_j'\rangle\langle\nu_j|$: $\begin{cases} \text{(1st quant.) replaces a } |\nu_j\rangle \text{ basis at the } j\text{-th place with } |\nu_j'\rangle \\ \text{(2nd quant.) } \left.\begin{array}{ll} (n_{\nu_j}, n_{\nu_j'}) \to (n_{\nu_j}-1, n_{\nu_j'}+1) & \text{if } \nu_j \neq \nu_j' \\ (n_{\nu_j}) \to (n_{\nu_j}) & \text{if } \nu_j = \nu_j' \end{array}\right\} \end{cases}$

done by $a^\dagger_{\nu_j'} a_{\nu_j}$

$a = b$ (boson), c (fermion)

$T_{tot} = \sum_{\nu'\nu} T_{\nu'\nu}\, a^\dagger_{\nu'} a_\nu$ (quadratic)

Two-particle operators: $V_{tot} = \frac{1}{2} \sum_{j \neq k} V_{jk}$

$V_{jk} = \sum_{\nu_j'} \sum_{\nu_k'} \sum_{\nu_j} \sum_{\nu_k} |\nu_j'\rangle |\nu_k'\rangle \overbrace{\int d\vec{r}\, d\vec{r}' \langle \nu_k' | \vec{r}'\rangle \langle \nu_j' | \vec{r}\rangle V(\vec{r} - \vec{r}') \langle \vec{r} | \nu_j\rangle \langle \vec{r}' | \nu_k\rangle}^{= V_{\nu_j' \nu_k' \nu_j \nu_k}} \langle \nu_k | \langle \nu_j |$

$V_{tot} = \sum_{\substack{\nu'\mu' \\ \nu\mu}} V_{\nu_j' \nu_k' \nu_j \nu_k}\, a^\dagger_{\nu'} a^\dagger_{\mu'} a_\mu a_\nu$ (quartic)

$|\nu\rangle\langle\nu| = a^\dagger_\nu |0\rangle\langle 0| a_\nu$ carries even # of fermionic operators

Change of basis

Two different complete single-particle basis sets: $\{|\nu_1\rangle, |\nu_2\rangle, \cdots\}$ $\{|\mu_1\rangle, |\mu_2\rangle, \cdots\}$

$$|\mu\rangle = \sum_\nu |\nu\rangle\langle\nu|\mu\rangle = \sum_\nu \langle\nu|\mu\rangle |\nu\rangle$$

$$|\mu\rangle = a_\mu^\dagger |0\rangle, \quad |\nu\rangle = a_\nu^\dagger |0\rangle$$

$$a_\mu^\dagger = \sum_\nu \langle\nu|\mu\rangle a_\nu^\dagger, \quad a_\mu = \sum_\nu \langle\mu|\nu\rangle a_\nu$$

① Same commutation relation holds:

$$[a_{\mu_1}, a_{\mu_2}^\dagger]_\mp = \sum_{\nu_1\nu_2} \langle\mu_1|\nu_1\rangle\langle\nu_2|\mu_2\rangle \underbrace{[a_{\nu_1}, a_{\nu_2}^\dagger]_\mp}_{=\delta_{\nu_1\nu_2}} = \underbrace{\sum_{\nu_1} \langle\mu_1|\nu_1\rangle\langle\nu_1|}_{=1}\mu_2\rangle = \langle\mu_1|\mu_2\rangle = \delta_{\mu_1\mu_2}$$

② Total number of particles do not change:

$$\sum_\mu a_\mu^\dagger a_\mu = \sum_\mu \sum_{\nu_1\nu_2} \langle\nu_1|\mu\rangle\langle\mu|\nu_2\rangle a_{\nu_1}^\dagger a_{\nu_2} = \sum_{\nu_1\nu_2} \underbrace{\langle\nu_1|\nu_2\rangle}_{=\delta_{\nu_1\nu_2}} a_{\nu_1}^\dagger a_{\nu_2} = \sum_{\nu_1} a_{\nu_1}^\dagger a_{\nu_1}$$

$$\sum_\mu |\mu\rangle\langle\mu| = 1$$

Example: non-interacting fermions

$$\mathcal{H} = \sum_{\nu\nu'} t_{\nu\nu'} c_\nu^\dagger c_{\nu'} \qquad \nu = (\vec{k},\sigma) \text{ or } (i,\sigma) \qquad t_{\nu\nu'} = [t]_{\nu\nu'} \qquad t^\dagger = t$$

Diagonalize: $t = U \varepsilon U^\dagger \qquad U = [\vec{u}_1\ \vec{u}_2\ \cdots] \qquad \varepsilon = \begin{pmatrix} \varepsilon_1 & & 0 \\ & \varepsilon_2 & \\ 0 & & \ddots \end{pmatrix} \qquad \varepsilon_1 \le \varepsilon_1 \le \varepsilon_3 \le \cdots$

$$\vec{u}_i^\dagger \vec{u}_j = \delta_{ij}$$

$$\mathcal{H} = \sum_\mu \varepsilon_\mu \gamma_\mu^\dagger \gamma_\mu \qquad \gamma_\mu^\dagger = \sum_\nu U_{\nu\mu} c_\nu^\dagger \qquad U_{\mu\nu} = \langle \nu | \mu \rangle = [\vec{u}_\mu]_\nu$$

Many-body energy eigenstate: $|\vec{n}\rangle = |n_{\mu=1}, n_{\mu=2}, \cdots\rangle \qquad \gamma_\mu^\dagger \gamma_\mu |\vec{n}\rangle = n_\mu |\vec{n}\rangle$

$$\mathcal{H}|\vec{n}\rangle = \underbrace{\left(\sum_\mu \varepsilon_\mu n_\mu\right)}_{=: E(\vec{n})} |\vec{n}\rangle$$

Ground state: $|n_1, n_2, \cdots, n_r, n_{r+1}, \cdots\rangle$ such that $n_\mu = 1$ for $\varepsilon_\mu < 0$, $n_\mu = 0$ for $\varepsilon_\mu > 0$,

$n_\mu = 0, 1$ for $\varepsilon_\mu = 0$

Ground-state energy: $E_G = \sum_{\varepsilon_\mu < 0} \varepsilon_\mu$

Ground-state degeneracy: $2^{\#\text{ of } \mu\text{'s such that } \varepsilon_\mu = 0}$

What if interacting?

Non-interacting: $\mathcal{H} = \sum_\mu \varepsilon_\mu c_\mu^\dagger c_\mu$

$|\vec{n}\rangle = |n_1, n_2, \cdots\rangle$

Interacting: $\mathcal{H} = \sum_\mu \varepsilon_\mu c_\mu^\dagger c_\mu + (\text{non-quadratic terms})$

$\sum_{\vec{n}} A_{\vec{n}} |\vec{n}\rangle$ often complicated!

Hilbert space dimension: $\left|\{|\vec{n}\rangle\}\right| = 2^{\#\text{ of basis}}$ "Exponential wall"

References

[Fetter2003], [Mahan2007] ← Classics (first editions were in 1971 & 1981)

[Bruss2004]

Note: In some literature, operators in second quantization are denoted with hat symbols, e.g., $\hat{c}_\nu$, $\hat{c}_\nu^\dagger$, not to be confused with numbers. The choice of putting hats depends on literature. In this handwritten lecture note, I wrote operators without hats to improve the readability.