2. Second quantization

N-particle state: $$|\psi\rangle = \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} (\pm 1)^{\pi} \, |\varphi_{\pi(1)}\rangle_{(1)} \otimes \dots \otimes |\varphi_{\pi(N)}\rangle_{(N)} \qquad (1)$$

single particle states

$$\Rightarrow |\varphi_i\rangle \in \mathcal{H}, \quad |\psi\rangle \in \underbrace{\mathcal{H} \otimes \dots \otimes \mathcal{H}}_{N \cdot \text{times}} = \mathcal{H}^N \qquad (2)$$

Problems with this formalism:

(i) Difficult to use for large N $(\sim 10^{23})$

(ii) Number of particles N is fixed $\rightarrow$ problematic for physical situations, where N is not known a priori or can change (e.g.: grandcanonical ensemble, superconductivity, ...)

$\Rightarrow$ Improoved formalism for quantum many-particle theory is required!

(i) Only relevant information in $|\psi\rangle$:

How often is a single-particle state $|i\rangle = |\varphi_i\rangle$ occupied?

$\Rightarrow$ $\boxed{\text{Occupation number}}$ $n_i = \begin{cases} 0, 1 & \text{for fermions} \\ 0, \dots, \infty & \text{for bosons} \end{cases}$

$\Rightarrow$ $|\psi\rangle$ is uniquely defined by the occupation numbers:

$$|\psi\rangle \triangleq |n_1, n_2, \dots\rangle \,, \quad \sum_{l=1}^{\infty} n_l = N \qquad (3)$$

$\hookrightarrow$ sum over all one-particle states

$\Rightarrow$ $\boxed{\text{Occupation number representation}}$

But: How can we deal with a variable number of particles?

$\boxed{\text{Reminder:}}$ Harmonic oscillator: $H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$

Ladder operators: $\begin{cases} a = \sqrt{\frac{m\omega}{2\hbar}}\, x + i\sqrt{\frac{1}{2m\omega\hbar}}\, p \\ a^+ = \sqrt{\frac{m\omega}{2\hbar}}\, x - i\sqrt{\frac{1}{2m\omega\hbar}}\, p \end{cases} \Leftrightarrow \begin{cases} x = \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^+) \\ p = -i\sqrt{\frac{m\omega\hbar}{2}}\,(a - a^+) \end{cases}$

It is easy to show that: $\cdot\ [a, a^+] = 1$ (consider $[p, x] = \frac{\hbar}{i}$!)

$\cdot\ H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 = \frac{\hbar\omega}{2}(aa^+ + a^+a) = \hbar\omega(a^+a + \frac{1}{2})$

$\Rightarrow\ [H, a^+] = \hbar\omega a^+ \qquad [H, a] = -\hbar\omega a$

For an eigenstate $|n\rangle$ of H ($H|n\rangle = E_n|n\rangle$):

$a^+|n\rangle$: $H(a^+|n\rangle) = a^+(\overbrace{H|n\rangle}^{E_n|n\rangle} + \hbar\omega|n\rangle) = (E_n + \hbar\omega)(a^+|n\rangle)$

$\Rightarrow a^+|n\rangle$ ... eigenstate with energy $E_n + \hbar\omega$

$a|n\rangle$: $H a|n\rangle = a(H|n\rangle - \hbar\omega|n\rangle = (E_n - \hbar\omega) a|n\rangle$

$\Rightarrow a|n\rangle$ ... eigenstate with energy $E_n - \hbar\omega$

For the ground state $|0\rangle$ with the ground state energy E_0 we have:

$a|0\rangle = 0$ (Otherwise the energy of $a|0\rangle$ would be $E_0 - \hbar\omega < E_0$)

$$H|0\rangle = \frac{\hbar\omega}{2}(a^+a + aa^+)|0\rangle = \frac{\hbar\omega}{2}[2a^+\underbrace{a|0\rangle}_{0} + 1|0\rangle] = \frac{\hbar\omega}{2}\cdot|0\rangle$$

$$\Rightarrow \boxed{E_0 = \frac{\hbar\omega}{2}}$$

All excited states can be generated by applying $(a^+)^n$ to $|0\rangle$:

$|n\rangle \sim (a^+)^n|0\rangle$, $E_n = \frac{\hbar\omega}{2}(2n+1)$

Normalization: $a^+|n\rangle = C|n+1\rangle \Rightarrow \langle n|\underbrace{aa^+}_{\frac{H}{\hbar\omega}+\frac{1}{2}}|n\rangle = C^2 = n+1$

$$\Rightarrow \boxed{\begin{aligned} a^+|n\rangle &= \sqrt{n+1}\,|n+1\rangle \\ a|n\rangle &= \sqrt{n}\,|n-1\rangle \end{aligned}}$$

Interpretation of the <u>ladder operators</u> a and a^+ :

a^+ ... increases the energy by a quantum $\hbar\omega$
a ... reduces the energy by a quantum $\hbar\omega$
a^+a ... $a^+a|n\rangle = n|n\rangle$ counts the number of quanta in state $|n\rangle$
$\Rightarrow a^+a = n$ .... number operator

$\Rightarrow$ an energy quantum $\hbar\omega$ can be interpreted as bosonic particle with energy $\hbar\omega$ (corresponds classically to frequency ω of the oscillator)

$\Rightarrow$ The state $|n\rangle$ contains n bosonic particles (corresponds classically to amplitude of the oscillator)

Interpretation of a and a^+

a^+ ... creation operator $\Rightarrow$ creates boson
a ... annihilation operator $\Rightarrow$ annihilates boson

<u>Example</u>: quanta of electromagnetic field: photons with energy $E = h\nu = \hbar\omega$

(ii) Hilbert space with variable number of particles:

$$F = \mathcal{H}^0 \oplus \mathcal{H}^1 \oplus \mathcal{H}^2 \otimes \ldots = \bigoplus_{n=0}^{\infty} \mathcal{H}^n \quad (4)$$

$\mathcal{H}$ ... one-particle Hilbert space

$\mathcal{H}^n = \underbrace{\mathcal{H} \otimes \mathcal{H} \otimes \ldots \otimes \mathcal{H}}_{n \text{ times}} \Rightarrow$ n-particle Hilbert sp.

F ... Fock space

How to change the particle number?

$|\psi\rangle = |n_1, n_2, .. n_i, \ldots\rangle \in \mathcal{H}^n$ (5) $\Rightarrow$ We define a creation operator c_i^+ (c.f. Harmonic oscillator)

$$\Rightarrow c_i^+ |\psi\rangle = (\underset{\text{Fermions}}{\overset{\text{Bosons}}{\pm}} 1)^{n_1 + \ldots + n_{i-1}} \sqrt{(n_i+1)^{\overset{\text{Bosons}}{\oplus}1}}\, |n_1, n_2, \ldots, n_i + 1\rangle \quad (6a)$$

Fermions: Integer division $\Rightarrow (n_i+1)^{-1} \equiv 0$ for $n_i \geq 1$

$$\Rightarrow c_i |\psi\rangle = (\pm 1)^{n_1 + \ldots + n_{i-1}} \sqrt{n_i}\, |n_1, n_2, \ldots, n_i - 1, \ldots\rangle \quad (6b)$$

$\hookrightarrow$ if $n_i = 0 \Rightarrow c_i |\psi\rangle = 0$

$c_i^\dagger$ ... creation operator
adds additional particle in state i

c_i ... annihilation operator
removes particle in state i

$$\begin{tikzcd}
0 & \mathcal{H}^0 \arrow[l, bend left, "c"] \arrow[r, bend left, "c^\dagger"] & \mathcal{H}^1 \arrow[l, bend left, "c"] \arrow[r, bend left, "c^\dagger"] & \mathcal{H}^2 \arrow[l, bend left, "c"] \arrow[r, bend left, "c^\dagger"] & \mathcal{H}^3 \arrow[l, bend left, "c"] \arrow[r, bend left, "c^\dagger"] & \dots \arrow[l, bend left, "c"]
\end{tikzcd}$$

(Note: $c_i |\psi\rangle$ vanishes if $|\psi\rangle$ does not contain the single-particle state $|\varphi_i\rangle$)

Remarks:

→ $\mathcal{H}^0 = \mathbb{C}$ contains no particles ⇒ Only state in $\mathcal{H}^0$: $|0,0,\dots\rangle$
⇒ „Vacuum": written as $|0\rangle$ or $|vac\rangle$.
↳ ! not the zero vector of $\mathcal{F}$!

→ All many particle states $|\psi\rangle \in \mathcal{F}$ can be generated by applying creation operators to the vacuum!

Commutator algebra of creation and annihilation operators

$\Rightarrow$ What is the relation between $c_i^{(+)} c_j^{(+)}$ and $c_j^{(+)} c_i^{(+)}$?

- $c_i^+ c_j^+ |\psi\rangle$ and $c_j^+ c_i^+ |\psi\rangle$ (see Eqs. (6)): $(i<j)$

$$c_i^+ c_j^+ |\psi\rangle = (\pm 1)^{n_1+\ldots+n_{j-1}} \sqrt{(n_j+1)^{\pm 1}}\; c_i^+ |n_1, \ldots, n_j+1, \ldots\rangle$$

$$= (\pm 1)^{n_i+\ldots+n_{j-1}} \sqrt{(n_i+1)^{\pm 1}} \sqrt{(n_j+1)^{\pm 1}}\; |n_1, \ldots, n_i+1, \ldots, n_j+1, \ldots\rangle \quad (7a)$$

$$c_j^+ c_i^+ |\psi\rangle = (\pm 1)^{n_1+\ldots+n_{i-1}} \sqrt{(n_i+1)^{\pm 1}}\; c_j^+ |n_1, \ldots, n_i+1, \ldots\rangle$$

$$= (\pm 1)^{(n_i+1)+\ldots+n_{j-1}} \sqrt{(n_j+1)^{\pm 1}} \sqrt{(n_i+1)^{\pm 1}}\; |n_1, \ldots, n_i+1, \ldots, n_j+1, \ldots\rangle \quad (7b)$$

$$\Rightarrow \quad c_i^+ c_j^+ |\psi\rangle = (-1)^{\overset{\text{Bosons}}{\oplus}}_{\underset{\text{Fermions}}{\ominus}}\; c_j^+ c_i^+ |\psi\rangle \Rightarrow$$

commutator

$$c_i^+ c_j^+ - c_j^+ c_i^+ = [c_i^+, c_j^+] = 0 \text{ for bosons} \quad (8)$$

$$c_i^+ c_j^+ + c_j^+ c_i^+ = \{c_i^+, c_j^+\} = 0 \text{ for fermions} \quad (9)$$

anticommutator

$\Rightarrow$ also valid for $i=j$! $\Rightarrow$ Fermions: $(c_i^+)^2 = 0$

↳ Pauli exclusion principle!

- $c_i c_j|\psi\rangle$ and $c_j c_i|\psi\rangle \Rightarrow$ analogous calculation as for $c_i^+ c_j^+|\psi\rangle$

$\Rightarrow$ $[c_i, c_j]=0$ (for bosons) and $\{c_i, c_j\}=0$ (for fermions) (10)

- $c_i^+ c_j|\psi\rangle$ and $c_j c_i^+|\psi\rangle$

→ for $\boxed{i \neq j}$ $\Rightarrow$ analogous calculation as for $c_i^+ c_j^+|\psi\rangle$ and $c_i c_j|\psi\rangle$:

$[c_i^+, c_j]=0$ (for bosons) and $\{c_i^+, c_j\}=0$ (for fermions) (11)

→ for $\boxed{i=j}$:

$$c_i^+ c_i|\psi\rangle = (\pm 1)^{n_1+\ldots+n_{i-1}} \sqrt{n_i}\, c_i^+ |n_1, \ldots, n_i-1, \ldots\rangle = n_i |n_1, \ldots, n_i, \ldots\rangle \quad (12a)$$

$$c_i c_i^+|\psi\rangle = (\pm 1)^{n_1+\ldots+n_{i-1}} \sqrt{(n_i+1)}^{\pm 1}\, c_i |n_1, \ldots, n_i+1, \ldots\rangle = (n_i+1) |n_1, \ldots, n_i, \ldots\rangle \quad (12b)$$

$\Rightarrow$ $[c_i, c_i^+]=1$ (for bosons) and $\{c_i^+, c_i\}=1$ (for fermions) (13)

<u>Note:</u> For fermionic state $|\psi\rangle$: Either $c_i^+ c_i|\psi\rangle=0$ (if $n_i=0$) or $c_i c_i^+|\psi\rangle=0$ (if $n_i=1$) !!

Summary: $[c_i^\dagger, c_j^\dagger] = [c_i, c_j] = 0$ and $[c_i, c_j^\dagger] = \delta_{ij}$ for bosons (14a)

$\{c_i^\dagger, c_j^\dagger\} = \{c_i, c_j\} = 0$ and $\{c_i, c_j^\dagger\} = \delta_{ij}$ for fermions (14b)

$c_i^\dagger c_i |\psi\rangle = n_i |\psi\rangle \Rightarrow \hat{n}_i = c_i^\dagger c_i$ ... number operator

$\Rightarrow$ $\hat{n}_i$ counts the number of particles in the single-particle state $|\varphi_i\rangle$ in the many-particle state $|\psi\rangle$.

Basis independence of the formalism:

$\Rightarrow$ Formalism is built on an (orthonormal) Basis $|i\rangle = |\varphi_i\rangle$ of the single-particle Hilbert space!

$\Rightarrow$ What happens, if we go a new single-particle basis $|\chi_j\rangle$?

$|\chi_i\rangle = \sum_j U_{ij} |\varphi_j\rangle$, U_{ij}... unitary transformation ($U^\dagger U = U U^\dagger = \mathbb{1}$)

$c_j^+ \ldots$ creates $|\varphi_j\rangle$, $d_i^+ \ldots$ creates $|\chi_i\rangle$ (15)

$\Rightarrow$ $d_i^+|0\rangle = |\chi_i\rangle = \sum_j U_{ij}|\varphi_j\rangle = \overbrace{\sum_j U_{ij} c_j^+}^{d_i^+}|0\rangle$ (16)

$\Rightarrow$ $\boxed{d_i^+ = U_{ij}\, c_j^+ \qquad d_i = U_{ji}^+\, c_j}$ (17) $\rightarrow$ Commutation relations for $d_i^{(+)}$?

$$\begin{cases} \underbrace{\{/[}_{\text{commutator/anticommutator}} d_i , d_j^+ \}/] = U_{ki}^+ U_{jl} \underbrace{\{/[c_k , c_l^+\}/]}_{\delta_{kl}} = U_{ki}^+ U_{jk} = \delta_{ij} & (18a) \\ \{/[d_i^+ , d_j^+\}/] = \{/[d_i , d_j\}/] = 0 & (18b) \end{cases}$$

$\Rightarrow$ Commutator algebra is invariant under basis transformation!!

Relation to wave function in first quantization:

1-particle wavefunction: $|\varphi_i\rangle = c_i^+|0\rangle$; in basis $|\chi_j\rangle$: $\varphi_i(j) = \langle 0|d_j c_i^+|0\rangle$

N-particle wave function: $|\varphi\rangle = c_1^+ \ldots c_n^+|0\rangle$; in basis $|\chi_j\rangle$: $\varphi_{1\ldots n}(j_1,\ldots,j_n) = \langle 0|d_{j_1} \ldots c_n^+|0\rangle$

Examples for different single-particle basis states:

-) position-spin bases: $|\varphi_i\rangle \Rightarrow |\vec{r}\sigma\rangle$ $\left(i \,\hat{=}\, (\vec{r},\sigma)\right)$
↳ continuous!

$c_i^{(+)} \rightarrow \underbrace{\psi_\sigma^{(+)}(\vec{r})}$ → field operator

$$\{[\psi_\sigma^{(+)}(\vec{r}), \psi_{\sigma'}^{(+)}(\vec{r}')\}|] = 0 \qquad \{/[\psi_\sigma(\vec{r}), \psi_{\sigma'}^{+}(\vec{r}')\}|] = \delta_{\sigma\sigma'}\, \delta^{(3)}(\vec{r}-\vec{r}') \quad (19)$$

δ-Funktion instead of Kronecker-delta!

Note: These (anti)commutation relations guarantee microcausality in relativistic quantum field theory!

$\rightarrow [A(t,\vec{r}), B(t',\vec{r}')] = 0$ for space-like distances $(t-t')^2-(\vec{r}-\vec{r}')^2 < 0$

Relation to wave function in 1st quantization: $\varphi_{i\sigma}(\vec{r}) = \langle 0|\psi_\sigma(\vec{r})c_i^+|0\rangle$

-) momentum-spin basis: $|\varphi_i\rangle \Rightarrow |\vec{k}\sigma\rangle \Rightarrow$ analogous to $|\vec{r}\sigma\rangle$
Transition from $\psi_\sigma(\vec{r}) \rightarrow \psi_\sigma(\vec{k})$: Fouriertransformation!

Operators in 2nd quantization:

How can we represent physical observables – i.e. Hermitian operators in 2nd quantization?

• 1-particle operator:

$$O_1 = \sum_{i=1}^{N} O_1^{(i)} \qquad \left[\text{e.g.: } \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} \quad \text{or} \quad \sum_{i=1}^{N} V(\vec{r}_i) \right]$$

↳ acts in one-particle Hilbert space of particle i!

⇒ Spectral representation: $O_1 = \sum_{i=1}^{N} \sum_{n,m} |\varphi_m\rangle_{(i)} \, {}_{(i)}\langle\varphi_m| O_1^{(i)} |\varphi_n\rangle_{(i)} \, {}_{(i)}\langle\varphi_n|$ (20)

⇒ How does O_1 act on N-particle state $|\psi\rangle = \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} (\pm 1)^{\pi} |\varphi_{\pi(1)}\rangle_{(1)} \otimes \ldots \otimes |\varphi_{\pi(N)}\rangle_{(N)}$

occupied states 1…N

↳ number of the particle

$$\Rightarrow O_1|\psi\rangle = \sum_{i=1}^{N} \sum_{n,m} \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} (\pm 1)^{\pi} \, {}_{(i)}\langle\varphi_m| O_1^{(i)} |\varphi_n\rangle_{(i)}$$

$$\times \, {}_{(i)}\langle\varphi_n|\varphi_{\pi(i)}\rangle_{(i)} \, |\varphi_{\pi(1)}\rangle \otimes \ldots \otimes |\varphi_m\rangle_{(i)} \otimes \ldots \otimes |\varphi_{\pi(N)}\rangle_{(N)} \quad (21)$$

$\Rightarrow \; {}_{(i)}\langle \varphi_n | \varphi_{\pi(i)} \rangle_{(i)} = \delta_{n\,\pi(i)}$ $\Rightarrow$ Only permutations $\pi \in S_N$ contribute for which $\pi(i) = n$!

$\Rightarrow \sum\limits_{\pi \in S_N} (\pm 1)^{\pi} \;\to\; \sum\limits_{\pi' \in S_{N-1}} (\pm 1)^{\pi'}$ $\quad \pi'$ … permutation of $1, \dots, n-1, n+1, \dots, N$

<u>Note:</u> ${}_{(i)}\langle \varphi_m | O_1^{(i)} | \varphi_n \rangle_{(i)}$ is independent of i!

$$\Rightarrow O_1 |\psi\rangle = \sum_m \sum_{n=1}^{N} \langle \varphi_m | O_1^{(1)} | \varphi_n \rangle \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} (\pm 1)^{\pi} |\varphi_1\rangle_{\pi(1)} \otimes \dots \otimes |\varphi_{n-1}\rangle_{\pi(n-1)} \otimes \boxed{|\varphi_m\rangle_{\pi(n)}} \otimes |\varphi_{n+1}\rangle_{\pi(n+1)} \otimes \dots \otimes |\varphi_N\rangle_{\pi(N)} \quad (22)$$

$\hookrightarrow \delta_{n\pi(1)} \to n \in (1, \dots, N)$: states $(1, \dots, N)$ are occupied in $|\psi\rangle$!

„new" state

$\hookrightarrow$

Occupied single particle states: $\underset{\text{in } |\psi\rangle}{(1, \dots, \boxed{n}, \dots, N)} \xrightarrow{O_1} \underset{\text{in } O_1|\psi\rangle}{(1, \dots, \boxed{m}, \dots, N)}$

$\Rightarrow O_1|\psi\rangle$ … N-particle state with $|\varphi_n\rangle$ replaced by $|\varphi_m\rangle$ with an amplitude $\langle \varphi_m | O_1^{(1)} | \varphi_n \rangle$!

$\Rightarrow$ $|\varphi_n\rangle$ anihilated $\Rightarrow c_n$
$|\varphi_m\rangle$ created $\Rightarrow c_m^+$ $\Big\} \Rightarrow$

$$\boxed{\underbrace{O_1}_{O_1 \text{ in } 2^{nd} \text{ quantization}} = \sum_{mn} \overbrace{\langle\varphi_m|\underbrace{O_1^{(1)}}_{O_1^{(1)} \text{ in } 1^{st} \text{ quantiz.}}|\varphi_n\rangle}^{\text{matrix element in } 1^{st} \text{ quantisation}} c_m^+ c_n} \quad (23)$$

Remarks:

$\rightarrow$ O_1 in 2^{nd} quantization independent on choice of bases $|\varphi_i\rangle$! ✓

$\rightarrow$ For an eigenbasis $\{|\varepsilon_n\rangle\}$ of $O_1^{(1)}$ we have: $\langle\varepsilon_m|O_1^{(1)}|\varepsilon_n\rangle = \varepsilon_n \delta_{nm}$

$$\Rightarrow O_1 = \sum_n \varepsilon_n c_n^+ c_n = \sum_n \varepsilon_n \hat{n}_n \quad (\hat{n}_n \text{... number operator})$$

$|\varphi_m\rangle \hat{=} c_m^+$ was originally on the left!!

$\rightarrow$ In principle we should write: $O_1 = \sum_{mn} c_m^+ \langle\varphi_m|O_1^{(1)}|\varphi_n\rangle c_n$

because in some cases c_m^+ and $\langle\varphi_m|O_1^{(1)}|\varphi_n\rangle$ do not commute!
(See the examples in the following)

Examples for O_1:

→ Kinetic energy: 1st quantization: $H_{kin} = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m}$ (24)

2nd quantization ⇒ we have to choose a one-particle basis!

* Position basis $|\vec{r}\rangle$: $\langle \vec{r}\,' | \frac{\vec{p}^{\,2}}{2m} | \vec{r} \rangle = -\frac{\hbar^2}{2m} \delta^{(3)}(\vec{r}-\vec{r}\,') \Delta_{\vec{r}}$ (25)

$\Rightarrow H_{kin} = -\frac{\hbar^2}{2m} \int_{\mathbb{R}^3} d^3r \; \psi^+(\vec{r}) \, \Delta \psi(\vec{r})$ ⇒ Order of terms important!

$\hookrightarrow \equiv \sum_m$ Laplace operator acts only on $\psi(\vec{r})$!

* Momentum basis $|\vec{p}\rangle$: $\langle \vec{p}\,' | \frac{\vec{p}^{\,2}}{2m} | \vec{p} \rangle = \delta^{(3)}(\vec{p}\,'-\vec{p}) \frac{\vec{p}^{\,2}}{2m}$ (26)

$\Rightarrow H_{kin} = \int_{\mathbb{R}^3} d^3p \; \frac{\vec{p}^{\,2}}{2m} \psi^+(\vec{p}) \psi(\vec{p})$ (27) ($\psi^{(+)}(\vec{p})$... field operator in momentum space)

→ External potential: $H_{ext} = \sum_{i=1}^{N} V(\vec{r}_i)$ (28)

* Position basis $|\vec{r}\rangle$: $H_{ext} = \int_{\mathbb{R}^3} d^3r \; \psi^+(\vec{r}) V(\vec{r}) \psi(\vec{r})$ (29)

• 2-particle operator:

$$O_2 = \sum_{i=1}^{N} \sum_{j=i+1}^{N} V_2^{(ij)} \qquad \left[\text{e.g.: } \frac{e^2}{4\pi\varepsilon_0} \sum_{i<j=1}^{N} \frac{1}{|\vec{r}_i - \vec{r}_j|} \right] \quad (30)$$

↳ acts in 2-particle Hilbert space of particles i and j!

⇒ analogous calculation as for one-particle operators:

1) Construct two-particle matrix elements for a given one-particle basis $|\varphi_i\rangle$:

$$\langle \varphi_{m_1} | \otimes \langle \varphi_{m_2} | \, V_2 \, | \varphi_{n_1} \rangle \otimes | \varphi_{n_2} \rangle$$

2) Represent O_2 via creation and annihilation operators:

$$\boxed{O_2 = \sum_{\substack{m_1 m_2 \\ n_1 n_2}} \frac{1}{2} \langle \varphi_{m_1} | \otimes \langle \varphi_{m_2} | \, V_2 \, | \varphi_{n_2} \rangle \otimes | \varphi_{n_1} \rangle \, c^{+}_{m_1} c^{+}_{m_2} c_{n_2} c_{n_1}} \quad (31)$$

↳ avoids double counting due to $m_1 \leftrightarrow m_2$ and $n_1 \leftrightarrow n_2$

<u>Example:</u> Electrons in a solid in 2^{nd} quantization:

$$H = \underbrace{\sum_{i=1}^{N}\left[\frac{\vec{p}_i^{\,2}}{2m} + \sum_{j=1}^{N_i} V(\vec{R}_j - \vec{r}_i)\right]}_{\text{One-particle part } H_0} + \underbrace{\frac{e^2}{4\pi\varepsilon_0}\sum_{i<j=1}^{N}\frac{1}{|\vec{r}_i - \vec{r}_j|}}_{\text{Two-particle part } U} \qquad (32)$$

H_0: N independent electrons with kinetic energy $\frac{\vec{p}_i^{\,2}}{2m}$ in the periodic potential $\sum_{j=1}^{N_i} V(\vec{R}_j - \vec{r}_i)$ of the lattice ions.
↳ lattice vector of a Bravais lattice!

U: Coulomb repulsion between the electrons.

H in second quantization using $\boxed{\text{position eigenbasis } |\vec{r}\rangle}$:

$$\boxed{\begin{aligned} H = &\sum_{\sigma}\int_{\mathbb{R}^3} d^3r\, \psi_\sigma^{+}(\vec{r})\left[-\frac{\hbar^2}{2m}\Delta + \sum_{j=1}^{N_i} V(\vec{R}_j - \vec{r})\right]\psi_\sigma(\vec{r}) \\ &\frac{1}{2}\sum_{\sigma\sigma'}\int_{\mathbb{R}^3} d^3r \int_{\mathbb{R}^3} d^3r'\, \frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{r} - \vec{r}'|}\,\psi_\sigma^{+}(\vec{r})\,\psi_{\sigma'}^{+}(\vec{r}')\,\psi_{\sigma'}(\vec{r}')\,\psi_\sigma(\vec{r}) \end{aligned}} \qquad (33)$$

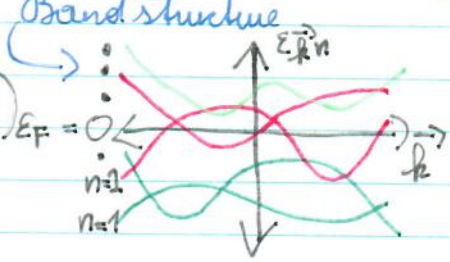
Fieldoperator $\psi_\sigma^{+}(\vec{r})$: generates electron with spin σ at $\vec{r}$!

Other possible choices of single-particle basis states:

* Bloch basis $|n\vec{k}\sigma\rangle$: Eigenstates of electrons in a periodic potential:

$\Rightarrow$ **Bloch states:** $\varphi_{\vec{k}n\sigma}(\vec{r}) = \langle \vec{r}|n\vec{k}\sigma\rangle$, $\quad H_0|n\vec{k}\sigma\rangle = \varepsilon_{n\vec{k}}\,|n\vec{k}\sigma\rangle$ (34)

n... Band index $\quad \vec{k}$... lattice momentum (in 1st Brillouin zone (BZ))



Matrix element of Coulomb interaction in Bloch basis:

$$V^{\vec{k}_1\ldots\vec{k}_4}_{n_1\ldots n_4} = \int_{\mathbb{R}^3} d^3r \int_{\mathbb{R}^3} d^3r' \, \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\vec{r}-\vec{r}\,'|} \, \varphi^*_{\vec{k}_1 n_1\sigma}(\vec{r})\, \varphi^*_{\vec{k}_2 n_2\sigma'}(\vec{r}\,')\, \varphi_{\vec{k}_3 n_3\sigma'}(\vec{r}\,')\, \varphi_{\vec{k}_4 n_4\sigma}(\vec{r}) \quad (35)$$

$\varphi_{\vec{k}n\sigma}(\vec{r}) = e^{i\vec{k}\vec{r}}\, u_{\vec{k}n}(\vec{r}) \approx e^{i\vec{k}\vec{r}}$ (nearly free electrons)

↳ lattice periodic $\Rightarrow u_{\vec{k}n}(\vec{r}+\vec{R}) = u_{\vec{k}n}(\vec{r})$, $\vec{R}$ = lattice vector

For nearly free electrons: Lattice potential $\sum_{j=1}^{N_i} V(\vec{R}_j - \vec{r}_i)$ „$\ll$" 1

$$\Rightarrow u_{\vec{k}n}(\vec{r}) \approx 1 \Rightarrow \psi_{\vec{k}n}(\vec{r}) \approx e^{i\vec{k}\vec{r}} \quad (36)$$

$\Rightarrow$ Interaction matrix:

$$U^{\vec{k}_1 \dots \vec{k}_4}_{n_1 \dots n_4} = \int_{\mathbb{R}^3} d^3r \int_{\mathbb{R}^3} d^3r' \, \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\vec{r}-\vec{r}'|} \, e^{i\vec{r}(\vec{k}_4-\vec{k}_1)} \, e^{i\vec{r}'(\vec{k}_3-\vec{k}_2)}$$

$$\stackrel{\vec{r}=\vec{r}'+\vec{r}''}{=} (2\pi)^3 \delta(\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}_4) \underbrace{\int_{\mathbb{R}^3} d^3r'' \frac{1}{|\vec{r}''|} e^{i\vec{r}''(\vec{k}_4-\vec{k}_1)}}_{4\pi(\vec{k}_4-\vec{k}_1)^{-2}} \quad (37)$$

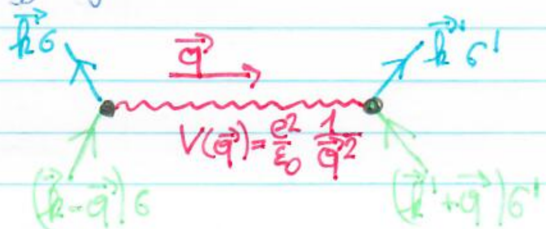
$\Rightarrow$ Relabel: $\vec{k}_1 = \vec{k}$ $\quad \vec{k}_2 = \vec{k}'$ $\quad \vec{k}_3 = \vec{k}'+\vec{q}$ $\quad \vec{k}_4 = \vec{k}-\vec{q}$

$$\boxed{H = \sum_{n\sigma}\sum_{\vec{k}} \varepsilon_{n\vec{k}} \psi^{+}_{n\sigma}(\vec{k}) \psi_{n\sigma}(\vec{k}) + \frac{1}{2} \sum_{\substack{\sigma\sigma' \\ n_1 \dots n_4}} \sum_{\vec{k}\vec{k}'\vec{q}} \boxed{\frac{e^2}{\varepsilon_0}\frac{1}{\vec{q}^2}} \boxed{\psi^{+}_{n_1\sigma}(\vec{k}) \psi^{+}_{n_2\sigma'}(\vec{k}')} \boxed{\psi_{n_3\sigma'}(\vec{k}'+\vec{q}) \psi_{n_4\sigma}(\vec{k}-\vec{q})}}$$

$\sum_{\vec{k}} = \frac{1}{V_{BZ}} \int_{BZ} d^3k$ ... normalized integral over 1st Brillouin zone!

V_{BZ} ... Volume of 1st Brillouin zone [$=(2\pi)^3$ for nearly free electrons]

Graphical illustration: (38)

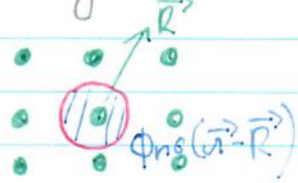


lattice vector

* Wannier basis $|n\vec{R}\sigma\rangle$: $\quad |n\vec{R}\sigma\rangle = \sum_{\vec{k}} e^{-i\vec{k}\vec{R}} |n\vec{k}\sigma\rangle$ (39)

⇒ $\boxed{\text{Tight binding}}$ description: Localized orbitals arround ion positions!

⇒ for almost localized systems: $\phi_{n\sigma}(\vec{r}-\vec{R}) = \langle \vec{r} | n\vec{R}\sigma\rangle$
approaches the atomic wave function (centered at $\vec{R}$)



$$H = \sum_{\sigma} \sum_{ij} \sum_{mn} -A_{ij}^{mn} c^{\dagger}_{im\sigma} c_{jn\sigma} + \sum_{\sigma\sigma'} \sum_{ijkl} \sum_{nmop} U_{ijkl}^{mnop} c^{\dagger}_{im\sigma} c^{\dagger}_{jn\sigma'} c_{ko\sigma'} c_{lp\sigma} \quad (40)$$

ij: site index
mn: band (orbital) index

- $A_{ij}^{mn} = -\int_{\mathbb{R}^3} d^3r\, \phi^*_{m\sigma}(\vec{r}-\vec{R}_i)\left(-\frac{\hbar^2}{2m}\Delta + \sum_{a=1}^{N_i} V(\vec{R}_a - \vec{r})\right)\phi_{n\sigma}(\vec{r}-\vec{R}_j) = -\delta_{mn} \sum_{\vec{k}} e^{i\vec{k}(\vec{R}_i - \vec{R}_j)} \varepsilon_{\vec{k}n}$ (41)

- $U_{ijkl}^{mnop} = \frac{1}{2} \int_{\mathbb{R}^3} d^3r \int_{\mathbb{R}^3} d^3r'\, \phi^*_{m\sigma}(\vec{r}-\vec{R}_i)\, \phi^*_{n\sigma'}(\vec{r}\,'-\vec{R}_j)\, \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\vec{r}-\vec{r}\,'|}\, \phi_{o\sigma'}(\vec{r}\,'-\vec{R}_k)\, \phi_{p\sigma}(\vec{r}-\vec{R}_l)$ (42)

Approximations:
→ Only one orbital at the Fermi level
→ Only local interaction
→ Only nearest neighbor hopping

⇒ $U = U_{iiii}^{nnnn}$, $A = A_{\langle ij\rangle}^{nn}$ ↳ nearest neighbours ⇒

$$\boxed{\text{Hubbard model (43)} \quad H = -A \sum_{\langle ij\rangle\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i c^{\dagger}_{i\uparrow} c_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow}}$$