01.31.23

We are interested in relating matrix element $\langle n_1, \ldots | F^{(1)} | n'_1, \ldots \rangle$ to the matrix elements of $\langle i | f^{(a)} | k \rangle$

$$\langle i | f^{(a)} | k \rangle = \int dr_a \, \psi_i^*(r_a) \, f^{(a)}(\hat{r}_a, \hat{p}_a) \, \psi_k(r_a)$$

(example : $n^{(a)}(R) = \delta(R - r_a) \Rightarrow \langle i | n^{(a)}(R) | k \rangle = \int dr_a \, \psi_i^*(r_a) \delta(R - r_a) \psi_k(r_a)$

$\langle i | n^{(a)}(R) | k \rangle = \psi_i^*(R) \psi_k(R)$)

Only one single-particle wave function, each from $\langle \ldots |$ and $| \ldots \rangle$ is involved non-trivially in the integration (once one uses

$$| n_1, n_2, \ldots \rangle = \sqrt{\frac{\prod_k n_k!}{N!}} \sum_{\{p'\}} \psi_{p_1}(r_1) \cdot \ldots \cdot \psi_{p_N}(r_N)$$

to evaluate $\langle \ldots | F | \ldots \rangle$). This is why at most one particle "moves" from one state (k) to another (i)

The only non-zero matrix elements :

$$n'_k = n_k - 1, \quad n'_i = n_i + 1, \quad n'_\ell = n_\ell \text{ for } \ell \neq i, k$$

or

$$n'_\ell = n_\ell \quad \forall \ell$$

Consider first the matrix elements with two of the occup. #s changing:

$$\langle n_1, \ldots, n_i, \ldots, n_k-1, \ldots | \hat{F}^{(1)} | n_1, \ldots, n_i-1, \ldots n_k, \ldots \rangle = \sqrt{n_i n_k}\, f_{ik}$$

where $\langle i|f^{(a)}|k\rangle = \int dr_a\, \varphi_i^*(r_a)\, f^{(a)}(\hat{r}_a, \hat{p}_a)\, \varphi_k(r_a)$

An example of $\hat{n}(R)$ to see the origin of $\sqrt{n_i n_k}$ factor.

$$\hat{n}(R) = \sum_a \hat{n}^a(R), \quad \hat{n}^a(R) = \delta(R - r_a) \; ; \quad f_{ik} = \varphi_i^*(R)\varphi_k(R).$$

$$\langle n_1, \ldots, n_i, \ldots, n_k-1, \ldots | \hat{n}(R) | n_1, \ldots, n_i-1, \ldots, n_k, \ldots \rangle$$

$$= \frac{1}{N!} \cdot \prod_{\ell \neq i,k} n_\ell! \cdot \underset{\substack{\uparrow \\ \text{from } \sum_a \ldots}}{N} \cdot \underbrace{\sqrt{n_i!(n_k-1)!}\sqrt{(n_i-1)!\, n_k!}} \quad \varphi_i^*(R)\varphi_k(R) \overbrace{\underbrace{\sum_{\{P\}_{bra}} \sum_{\{P\}_{ket}}}_{\text{over } N-1 \text{ particles}} \delta_{bra,ket}}^{\frac{(N-1)!}{\prod_{\ell \neq i,k} n_\ell!\,(n_k-1)!(n_i-1)!}}$$

$$\sqrt{n_i!(n_k-1)!}\sqrt{(n_i-1)!\, n_k!} = \sqrt{n_i n_k}\,(n_k-1)!(n_i-1)!$$

$$\frac{1}{N!} \cdot \prod_{\ell \neq i,k} n_\ell! \cdot N \cdot \sqrt{n_i!(n_k-1)!}\sqrt{(n_i-1)!\, n_k!} = \prod_{\ell \neq i,k} n_\ell! \cdot \frac{(n_k-1)!(n_i-1)!}{(N-1)!} \cdot \sqrt{n_i n_k}$$

$$\prod_{\ell \neq i,k} n_\ell! \cdot \frac{(n_k-1)!(n_i-1)!}{(N-1)!} \underbrace{\sum_{\{P\}_{bra}} \sum_{\{P\}_{ket}}}_{\text{over } N-1 \text{ particles}} \delta_{bra,ket} = \prod_{\ell \neq i,k} n_\ell! \cdot \frac{(n_k-1)!(n_i-1)!}{(N-1)!} \cdot \frac{(N-1)!}{\prod_{\ell \neq i,k} n_\ell!\,(n_k-1)!(n_i-1)!} = 1$$

thus,

$$\langle n_1, \ldots, n_i, \ldots, n_k-1, \ldots | \hat{n}(R) | n_1, \ldots, n_i-1, \ldots, n_k, \ldots \rangle = \sqrt{n_i n_k}\; \varphi_i^*(R)\varphi_k(R).$$

$$\boxed{\begin{cases} \langle n_1, \ldots, n_i, \ldots, n_k-1, \ldots | \hat{F}^{(1)} | n_1, \ldots, n_i-1, \ldots n_k, \ldots \rangle = \sqrt{n_i n_k}\, f_{ik}^{(1)} \\ \langle n_1, \ldots, n_i, \ldots n_k, \ldots | \hat{F}^{(1)} | n_1, \ldots n_i, \ldots n_k, \ldots \rangle = \sum_{i=1}^{\infty} n_i f_{ii}^{(1)} \\ f_{ik}^{(1)} = \int dr\, \varphi_i^*(r)\, f^{(1)}\, \varphi_k(r) \equiv \langle i|f^{(1)}|k\rangle \end{cases}}$$

Reading:
Eq. (64.2) in LL v.3

details: Fetter & Walecka, Ch. 1

Introduce annihilation operator $\hat{a}_i$ acting on $|n_1, n_2, \ldots, n_i, \ldots\rangle$:

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

The only non-zero matrix element of $\hat{a}_i$ is

$$\langle n_1, \ldots n_i - 1, \ldots | \hat{a}_i | n_1, \ldots, n_i, \ldots\rangle = \sqrt{n_i}$$

abbreviate to

$$\begin{cases} \langle n_i - 1 | \hat{a}_i | n_i \rangle = \sqrt{n_i} \\ \langle n_i | \hat{a}_i^+ | n_i - 1\rangle = \langle n_i - 1 | \hat{a}_i | n_i \rangle^* = \sqrt{n_i} \end{cases}$$

a_i^+ : creation operator (of a particle in state i)

$$a_i^+ |n_1, n_2, \ldots, n_i, \ldots\rangle = \sqrt{n_i + 1}\, |n_1, n_2, \ldots n_i + 1, \ldots\rangle$$

Consider

$$a_i^+ a_i |n_1, \ldots, n_i, \ldots\rangle = a_i^+ \sqrt{n_i}\, |n_1, \ldots, n_i - 1, \ldots\rangle = n_i\, |n_1, \ldots, n_i, \ldots\rangle$$

($\hat{a}_i^+ \hat{a}_i$: operator of particle # in state i)

$$\hat{a}_i \hat{a}_i^+ |n_1, \ldots, n_i, \ldots\rangle = (n_i + 1)\, |n_1, \ldots, n_i, \ldots\rangle$$

$$\hat{a}_i \hat{a}_i^+ - \hat{a}_i^+ \hat{a}_i = 1 \qquad \text{(regardless } n_i)$$

Generalizing for $i \neq k$:

$$\hat{a}_i \hat{a}_k^+ - \hat{a}_k^+ \hat{a}_i = 0 \qquad (i \neq k)$$

$$\hat{a}_i \hat{a}_k - \hat{a}_k \hat{a}_i = 0 \qquad (\text{any } i, k)$$

$$\boxed{[\hat{a}_i, \hat{a}_k^+] = \delta_{ik}, \quad [\hat{a}_i, \hat{a}_k] = 0 \qquad (\forall\, i, k)}$$

Using the defs. of $a_i, \hat{a}_i^+$ we may re-write $F^{(1)}$ so its action on Fock space becomes evident:

$$\boxed{\hat{F}^{(1)} = \sum_{ik} f_{ik}^{(1)} \hat{a}_i^+ \hat{a}_k \,, \qquad f_{ik}^{(1)} = \langle i | f^{(1)} | k \rangle}$$

Generalization on a "2-particle" operator, such as pair interaction potential $\quad (\hat{f}_{ab}^{(2)} = V(r_a - r_b))$

$$\hat{F}^{(2)} = \sum_{a>b} \hat{f}_{ab}^{(2)} = \frac{1}{2}\sum_{a,b} \hat{f}_{ab}^{(2)} - \frac{1}{2}\sum_a \hat{f}_{aa}^{(2)}$$

$$F^{(2)} = \frac{1}{2}\sum_{i,k,l,m} \langle ik | f^{(2)} | lm \rangle a_i^+ a_k^+ a_m a_l$$

$$\langle ik | f^{(2)} | lm \rangle = \int dr_1 \int dr_2 \, \psi_i^*(r_1) \psi_k^*(r_2) \hat{f}^{(2)}(\hat{r}_1, \hat{p}_1; \hat{r}_2, \hat{p}_2) \psi_l(r_1) \psi_m(r_2)$$

$$\hat{\mathcal{H}} = \sum_a \hat{\mathcal{H}}_a^{(1)} + \sum_{a>b} V(\bar{r}_a, \bar{r}_b) \,, \quad \text{with } \hat{\mathcal{H}}_a^{(1)} = -\frac{\hbar^2}{2m}\nabla^2 + U(\bar{r}_a)$$

In second quantization:

$$\hat{\mathcal{H}} = \sum_{ik} \langle i | \mathcal{H}^{(1)} | k \rangle a_i^+ a_k + \frac{1}{2}\sum_{i,k,l,m} \langle ik | \hat{V} | lm \rangle a_i^+ a_k^+ a_m a_l$$

$$\hat{N} = \sum_i a_i^+ a_i \;; \qquad [\hat{N}, \hat{\mathcal{H}}] = 0$$

(particle # conservation)

The wave function $|n_1, n_2, \dots\rangle$ can be represented by action of creation operators on vacuum $|0\rangle$

$$|n_1, n_2, \dots\rangle = \frac{1}{\sqrt{n_1! n_2! \dots}} (a_1^+)^{n_1} (a_2^+)^{n_2} \dots |0\rangle$$

(recall that $a_i^+ |n_1, .. n_i, ..\rangle = \sqrt{n_i+1}\, |n_1, ..., n_i+1, ...\rangle$

$$(a_i^+)^{n_i} |0\rangle = (a_i^+)^{n_i-1} a_i^+ |0\rangle = (a_i^+)^{n_i-1} \sqrt{1}\, |1\rangle = (a_i^+)^{n-2} \sqrt{2}\cdot\sqrt{1}\, |2\rangle$$
$$= \ldots = \sqrt{n_i!}\, |n_i\rangle\ )$$

$$|N, 0, \ldots 0\rangle = \frac{1}{\sqrt{N!}} (a_0^+)^N |0\rangle$$

In real space : $\Psi = \varphi_0(r_1)\, \varphi_0(r_2) \ldots \varphi_0(r_N)$

02.02.23

3.2. Fermions (LL v.3 §65)

Order one-particle states once and for all.

Consider a "single-body" operator, $\hat{F}^{(1)} = \sum_a \hat{f}_a^{(1)} = \sum_a f(\hat{r}_a, \hat{p}_a)$

The only non-zero elements of $\hat{F}$ in the basis of Fock states involve $\{n_i'\} = \{n_i\}$ (no change in occupations) or shift one particle from a state i to a state k: $n_i' = n_i \pm 1$, $n_k' = n_k \mp 1$ (all n's are 0 or 1)

Direct calculation shows:

$$\begin{cases} \langle \ldots 1_i, \ldots, 0_k \ldots | \hat{F}^{(1)} | \ldots 0_i, \ldots, 1_k, \ldots \rangle = \langle i | f^{(1)} | k\rangle \cdot (-1)^{\Sigma(i+1, k-1)}, & i<k \\ \langle \ldots, 0_k, \ldots 1_i \ldots | \hat{F}^{(1)} | \ldots 1_k, \ldots, 0_i, \ldots\rangle = \langle i | f^{(1)} | k \rangle \cdot (-1)^{\Sigma(k+1, i-1)}, & i>k \end{cases}$$

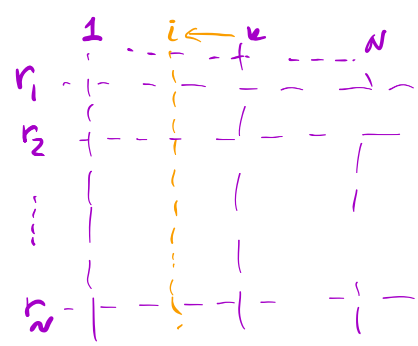
Here $|\ldots, 0_i, \ldots, 1_k \ldots\rangle = |n_1, n_2, \ldots, n_i = 0, \ldots, n_k = 1, \ldots\rangle$

(One may use properties of det to check the relations, and figure out $\Sigma(m,q)$)

$$\Sigma(m,q) = \sum_{\lambda=m}^{q} n_\lambda, \quad q \geq m$$

$$\Sigma(m,q) \overset{\text{def}}{=} 0 \quad \text{for } q<m$$

det :



Diagonal elements:

occup. number (0 or 1)

$$\langle n_1, \dots | F^{(1)} | n_1, \dots \rangle = \sum_{i=1}^{\infty} \langle i | f^{(1)} | i \rangle n_i$$

position of state (ordered once and for all)

Introduce operators a^+, a as matrices between the basis Fock states with the non-zero matrix elements:

$$\langle 0_i | \hat{a}_i | 1_i \rangle = \langle 1_i | \hat{a}_i^+ | 0_i \rangle = (-1)^{\Sigma(1, i-1)}$$

Use this relation to evaluate

$$\begin{cases} \langle 1_i, 0_k | \hat{a}_i^+ \hat{a}_k | 0_i, 1_k \rangle = (-1)^{\Sigma(i+1, k-1)} & i<k \\ \langle 1_i\, 0_k | \hat{a}_k \hat{a}_i^+ | 0_i, 1_k \rangle = -(-1)^{\Sigma(i+1, k-1)}, & i<k \end{cases}$$

$i<k$

Similar, at $k<i$ one gets these relations with $\Sigma(i+1, k-1) \to \Sigma(k+1, i-1)$

$$a_i^+ a_k + a_k a_i^+ = 0, \qquad i \neq k$$

$$\langle n_i | \hat{a}_i^+ \hat{a}_i | n_i \rangle = n_i, \qquad \langle n_i | a_i a_i^+ | n_i \rangle = 1 - n_i$$

(check directly from def of $a, \hat{a}$)

$$\hat{a}_i \hat{a}_i^+ + \hat{a}_i^+ \hat{a}_i = 1$$

Therefore

$$a_i^+ a_k + a_k a_i^+ = \delta_{ik}, \text{ or } \{a_i^+, a_k\} = \delta_{ik}$$

(Here $\{\hat{A}, \hat{B}\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$, anticommutator)

Similarly one gets:

$$a_i a_k + a_k a_i = 0, \text{ or } \{a_i, a_k\} = 0 \qquad (\forall i, k)$$

Using the creation and annihilation operators we may write $\hat{F}^{(1)}$ in the second-quant. rep.:

$$\hat F^{(1)} = \sum_{i,k} \langle i | f^{(1)} | k \rangle a_i^+ a_k$$

Now we derive for 2-body operators:

$$\hat F^{(2)} = \sum_{a>b} f^{(2)}_{ab} \Rightarrow \hat F^{(2)} = \frac{1}{2} \sum_{iklm} \langle ik | f^{(2)} | lm \rangle a_i^+ a_k^+ a_m a_l$$

(normal order of operators a^+, a)

with

$$\langle ik | f^{(2)} | lm \rangle = \int dr_1 \int dr_2\, \psi_i^*(r_1) \psi_k^*(r_2)\, \hat f^{(2)}(\hat r_1, \hat p_1; \hat r_2, \hat p_2)\, \psi_l(r_1) \psi_m(r_2)$$

The "two-body" operators in second quantization:

$$\hat F^{(2)} = \sum_{a>b} \hat f^{(2)}_{ab} = \frac{1}{2} \sum_{a,b} f^{(2)}(r_a, r_b) - \frac{1}{2} \sum_a f(\hat r_a, \hat r_a)$$

$$\hat F^{(2)} = \frac{1}{2} \sum_{a,b} \int dR_1 \int dR_2\, \underbrace{\delta(R_1 - r_a)}_{\sum_a} f(R_1, R_2) \underbrace{\delta(R_2 - r_b)}_{\sum_b}$$

$$- \frac{1}{2} \sum_a \int dR\, \delta(R - r_a)\, f(R, R)$$

$$= \frac{1}{2} \int dR_1 \int dR_2\, f(R_1, R_2) \sum_a \delta(R_1 - r_a) \sum_b \delta(R_2 - r_b)$$

$$- \frac{1}{2} \int dR\, f(R, R) \sum_a \delta(R - r_a)$$

$$= \frac{1}{2} \int dR_1 \int dR_2\, f(R_1, R_2)\, \hat n(R_1)\, \hat n(R_2) - \frac{1}{2} \int dR\, f(R, R)\, \hat n(R)$$

Use the "one-body" operators $\hat n(R)$ in second-quantized form:

$$\hat n(R_1) = \sum_{m,n} \psi_m^*(R_1) \psi_n(R_1)\, a_m^+ a_n$$

(recall $\langle m | \hat n(R) | n \rangle = \psi_m^*(R) \psi_n(R)$)

$$\hat n(R_2) = \sum_{k,l} \psi_k^*(R_2) \psi_l(R_2)\, a_k^+ a_l$$

$$\hat n(R_1)\, \hat n(R_2) \longrightarrow a_m^+ a_n a_k^+ a_l$$

① Check that $a_m^+ a_n a_k^+ a_l = a_m^+ a_k^+ a_l a_n + \delta_{nk}\, a_m^+ a_l$ (for bosons or fermions)

② use $\sum_{nk} \delta_{nk}\, \psi_k^*(R_2) \psi_n(R_1) = \delta(R_1 - R_2)$

③ see the cancellation of $\int dR\, f(R,R)\, \hat n(R)$ upon normal ordering.

$$\hat{\mathcal{H}} = \sum_a \hat{\mathcal{H}}_a^{(1)} + \sum_{a>b} V(\vec{r}_a, \vec{r}_b), \quad \text{with } \hat{\mathcal{H}}_a^{(1)} = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}_a)$$

In second quantization:

$$\hat{\mathcal{H}} = \sum_{ik} \langle i|\mathcal{H}^{(1)}|k\rangle a_i^+ a_k + \frac{1}{2}\sum_{i,k,l,m} \langle ik|\hat{V}|lm\rangle a_i^+ a_k^+ \hat{a}_m \hat{a}_l$$

order matters !

$$\langle i|\mathcal{H}^{(1)}|k\rangle = \int dr_1 \, \psi_i^*(r_1)\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}_a)\right)\psi_i(r_1)$$

$$\langle ik|\hat{V}|lm\rangle = \int dr_1 \int dr_2 \, \psi_i^*(r_1)\psi_k^*(r_2) V(r_1, r_2)\psi_l(r_1)\psi_m(r_2)$$

$$\hat{N} = \sum_i a_i^+ a_i, \quad [\hat{N}, \hat{\mathcal{H}}] = 0$$

GS wave function for non-interacting fermions:

$$|GS\rangle = |\underbrace{1, 1, 1 \ldots 1}_{N \text{ (total \# of particles)}}, 0\,0\,0\rangle = \prod_{E_i \leq E_F} a_i^+ |0\rangle$$

02.03.23

3.3. Field operators

We may justify the term "second quantization".

Introduce:

$$\hat{\Psi}(\vec{r}) = \sum_i \psi_i(\vec{r})\hat{a}_i, \quad \hat{\Psi}^+(\vec{r}) = \sum_i \psi_i^*(\vec{r})\hat{a}_i^+ \quad \text{(field operators)}$$

($\psi_i(\vec{r})$ form full orthonormal basis)

Commutation relations for $\hat{\Psi}$, $\hat{\Psi}^+$:

$$\hat{\Psi}(\vec{r}_1)\hat{\Psi}^+(\vec{r}_2) \underset{\text{bosons}}{\overset{\text{fermions}}{\pm}} \hat{\Psi}^+(\vec{r}_2)\hat{\Psi}(\vec{r}_1) = \sum_i \psi_i(\vec{r}_1)\hat{a}_i \sum_j \psi_j^*(\vec{r}_2)\hat{a}_j^+ \pm \sum_j \psi_j^*(\vec{r}_2)\hat{a}_j^+$$

$$\times \sum_i \psi_i(\vec{r}_1)\hat{a}_i = \sum_{ij} \psi_i(\vec{r}_1)\psi_j^*(\vec{r}_2)\left(\hat{a}_i\hat{a}_j^+ \underset{\text{bosons}}{\overset{\text{fermions}}{\pm}} a_j^+ a_i\right) = \sum_{ij} \delta_{ij} \psi_i(\vec{r}_1)\psi_j^*(\vec{r}_2)$$

$$= \sum_i \psi_i(\vec{r}_1)\psi_i^*(\vec{r}_2) = \delta(\vec{r}_1 - \vec{r}_2)$$

$$\begin{cases} \hat\psi(\vec r_1)\,\hat\psi^+(\vec r_2) \underset{\text{bosons}}{\overset{\text{fermions}}{\pm}} \hat\psi^+(\vec r_2)\,\psi(\vec r_1) = \delta(\vec r_1 - \vec r_2) \\ \hat\psi(r_1)\,\hat\psi(r_2) \underset{b}{\overset{f}{\pm}} \hat\psi(r_2)\,\hat\psi(r_1) = 0 \end{cases}$$

$$\hat{\mathcal{H}} = \int d\vec r \left\{ -\frac{\hbar^2}{2m} \hat\psi^+(\vec r)\, \nabla^2 \hat\psi(\vec r) + \hat\psi^+(\vec r)\, U(\vec r)\, \psi(\vec r) \right\}$$

$$+ \frac{1}{2} \int dr_1 \int dr_2\; \hat\psi^+(\vec r_1)\, \hat\psi^+(\vec r_2)\, V(\vec r_1, \vec r_2)\, \hat\psi(\vec r_2)\, \hat\psi(r_1)$$

$$\hat n(\vec r) = \hat\psi^+(\vec r)\,\hat\psi(\vec r) \;; \qquad \hat N = \int d\vec r\; \hat n(\vec r) = \int d\vec r\; \hat\psi^+(\vec r)\,\hat\psi(\vec r)$$

Particles with spin:

$$\hat\psi(\vec r) \longrightarrow \hat\psi(\vec r, \sigma) \equiv \hat\psi_\sigma(\vec r)$$

$$V = \frac{1}{2} \sum_{\sigma_1 \sigma_2} \int dr_1 \int dr_2\; \hat\psi^+_{\sigma_1}(r_1)\, \hat\psi^+_{\sigma_2}(r_2)\, V(r_1, r_2)\, \hat\psi_{\sigma_2}(r_2)\, \hat\psi_{\sigma_1}(r_1)$$

(spin-conserving interaction)

3.4. Change of the one-particle basis in second quantization

Two bases: $|\psi_\mu\rangle$ and $|\tilde\varphi_i\rangle$

The matrix elements of a single-particle operator:

$$f^{(1)}_{\mu\nu} = \langle \psi_\mu | \hat f^{(1)} | \psi_\nu \rangle \;; \qquad \tilde f^{(1)}_{ik} = \langle \tilde\varphi_i | \hat f^{(1)} | \tilde\varphi_k \rangle$$

The requirement that for any operator $\hat F^{(1)}$:

$$\hat F^{(1)} = \sum_{\mu\nu} f^{(1)}_{\mu\nu} \underbrace{a^+_\mu a_\nu}_{\substack{\text{operators defined in old} \\ \text{basis}}} = \sum_{ik} \tilde f^{(1)}_{ik} \underbrace{\tilde a^+_i \tilde a_k}_{\substack{\text{operators defined in} \\ \text{new basis}}} \qquad \text{is valid}$$

Satisfied with :

$$\tilde a_i = \sum_\nu \langle \tilde\varphi_i | \psi_\nu \rangle a_\nu \;; \qquad \tilde a^+_k = \sum_\mu \langle \tilde\varphi_k | \psi_\nu \rangle^* a^+_\mu$$

(Use $\sum_k |\tilde{\varphi}_k\rangle\langle\tilde{\varphi}_k| = \hat{I}$ to show this)

$\langle\tilde{\varphi}_i|\varphi_\nu\rangle = S_{i\nu}$ – unitary matrix $\Rightarrow$ the commutation relations are preserved in the new basis

$$[\tilde{a}_i, \tilde{a}_j^+]_{\pm} = \sum_{\nu_1\nu_2} S_{i\nu_1} S^+_{\nu_2 j} [a_{\nu_1}, a^+_{\nu_2}]_{\pm} = \sum_{\nu_1\nu_2} S_{i\nu_1}\delta_{\nu_1\nu_2} S^+_{\nu_2 j}$$

$\pm$ ← fermions; ↑ bosons

$$= \sum_{\nu_1} S_{i\nu_1} S^+_{\nu_1 j} = \delta_{ij}$$, same as $[a_{\nu_1}, a^+_{\nu_2}]_{\pm} = \delta_{ij}$.

(canonical transformation)

The particle # is conserved:

$$\sum_i \tilde{a}_i^+\tilde{a}_i = \sum_\mu a_\mu^+ a_\mu$$

3.5. Momentum representation of field operators

(use of plane-wave basis)

$$\hat{\psi}^+(\vec{r}) = \frac{1}{\sqrt{L^3}}\sum_{\vec{k}} e^{-i\vec{k}\vec{r}} a^+_{\vec{k}}, \qquad \hat{\psi}(\vec{r}) = \frac{1}{\sqrt{L^3}}\sum_{\vec{k}} e^{i\vec{k}\vec{r}} a_{\vec{k}}$$

(periodic boundary conditions for a cube $L\times L\times L$)

Operator of particle density

$$\hat{n}(\vec{r}) = \hat{\psi}^+(\vec{r})\hat{\psi}(\vec{r}) = \frac{1}{L^3}\sum_{\vec{k}_1\vec{k}_2} e^{i(\vec{k}_2-\vec{k}_1)\vec{r}} a^+_{\vec{k}_1} a_{\vec{k}_2}$$

$$= \frac{1}{L^3}\sum_{\vec{q}} e^{i\vec{q}\vec{r}} \sum_{\vec{k}_1} a^+_{\vec{k}_1} a_{\vec{k}_1+\vec{q}} \equiv \frac{1}{L^3}\sum_{\vec{q}} e^{i\vec{q}\vec{r}}\hat{n}(\vec{q})$$ (introduced $\vec{q} = \vec{k}_2 - \vec{k}_1$)

Fourier component of the particle density operator

$$\hat{n}(\vec{q}) \equiv \sum_k a^+_{\vec{k}} a_{\vec{k}+\vec{q}}$$

(Particles with spin; operator of density of particles in the spin state σ:

$$\hat{n}_\sigma(\bar{r}) = \frac{1}{L^3}\sum_q e^{i\bar{q}\bar{r}} n_\sigma(\bar{q}),\ n_\sigma(\bar{q}) = \sum_{\bar{k}} a^+_{\bar{k}\sigma} a_{\bar{k}+\bar{q}\sigma})$$

(useful if spin is a conserved quantity)

Next: we look at the pair interaction in a transl.-inv. system and show that

$$\hat{V} = \frac{1}{2L^3}\sum_{\bar{k}_1\bar{k}_2\bar{q}} V(\bar{q})\, a^+_{\bar{k}_1+\bar{q}} a^+_{\bar{k}_2-\bar{q}} a_{\bar{k}_2} a_{\bar{k}_1} \quad ; \quad V(\bar{q}) \equiv V_{\bar{q}} = \int d\bar{r}\, e^{i\bar{q}\bar{r}}\, V(\bar{r})$$

$$\hat{V} = \frac{1}{2}\int d\vec{r}_1 d\vec{r}_2\ \hat{\varphi}^+(\bar{r}_1)\hat{\varphi}^+(\bar{r}_2) V(\bar{r}_1-\bar{r}_2)\hat{\varphi}(\bar{r}_2)\hat{\varphi}(\bar{r}_1)$$

$$= \frac{1}{2}\cdot\frac{1}{L^6}\cdot\sum_{\substack{\bar{k}_1\bar{k}_2\\ \bar{k}_3\bar{k}_4}}\int d\vec{r}_1 d\vec{r}_2\ V(\vec{r}_1-\vec{r}_2)\, e^{i(\bar{k}_1\bar{r}_1+\bar{k}_2\bar{r}_2-\bar{k}_3\bar{r}_1-\bar{k}_4\bar{r}_2)}\ a^+_{\bar{k}_3}a^+_{\bar{k}_4}a_{\bar{k}_2}a_{\bar{k}_1}$$

$$\bar{k}_1\bar{r}_1+\bar{k}_2\bar{r}_2-\bar{k}_3\bar{r}_1-\bar{k}_4\bar{r}_2 = (\bar{k}_1-\bar{k}_3)r_1+(\bar{k}_2-\bar{k}_4)\bar{r}_2 = (\bar{k}_1-\bar{k}_3+\bar{k}_2-\bar{k}_4)\bar{r}_1 + (\bar{k}_2-\bar{k}_4)(\bar{r}_2-\bar{r}_1)$$

Introduce $\vec{r} = \bar{r}_2 - \bar{r}_1$

$$\int d\vec{r}_1 d\vec{r}_2\ V(\vec{r}_1-\vec{r}_2)\, e^{i(\bar{k}_1\bar{r}_1+\bar{k}_2\bar{r}_2-\bar{k}_3\bar{r}_1-\bar{k}_4\bar{r}_2)}$$

$$= \int_{L^3} d\bar{r}_1\, e^{i(\bar{k}_1-\bar{k}_3+\bar{k}_2-\bar{k}_4)\bar{r}_1}\int d\vec{r}\, V(\bar{r})\, e^{i(\bar{k}_2-\bar{k}_4)\bar{r}} = L^3\,\delta_{\bar{k}_1+\bar{k}_2,\,\bar{k}_3+\bar{k}_4}\cdot V(\bar{q})$$

We introduced here the transferred momentum: $\vec{q} = \vec{k}_2-\vec{k}_4 = \bar{k}_3-\bar{k}_1$,

$$V(\vec{q}) \equiv V_{\vec{q}} = \int d\bar{r}\, e^{i\bar{q}\bar{r}}V(\bar{r})$$

$$\hat{V} = \frac{1}{2L^3}\sum_{\bar{k}_1\bar{k}_2\bar{q}} V(\vec{q})\, a^+_{\bar{k}_1+\bar{q}} a^+_{\bar{k}_2-\bar{q}} a_{\bar{k}_2} a_{\bar{k}_1}.$$

Example: two-body scattering amplitude

T-matrix: $\hat{T} = \hat{V} + \hat{V}\hat{G}_0\hat{V} + \ldots,\quad G_0 = \dfrac{1}{E-\hat{H}_0}\ ;\quad \hat{H} = \hat{H}_0 + \hat{V}$

Born approx.: $\hat{T}^{(1)} = \hat{V}$

Initial state: two particles with momenta $\vec{p}_1, \vec{p}_2$ (and $\vec{p}_1 \neq \vec{p}_2$)

$$|\vec{p}_1 \vec{p}_2 \rangle = a^+_{\vec{p}_1} a^+_{\vec{p}_2} |0\rangle$$

Final state:

$$|\vec{p}_1 + \vec{Q}, \vec{p}_2 - \vec{Q} \rangle = a^+_{\vec{p}_1+\vec{Q}} \, a^+_{\vec{p}_2-\vec{Q}} |0\rangle$$

Scattering amplitude

$$\langle \vec{p}_1+\vec{Q}, \vec{p}_2 - \vec{Q} \,|\, \hat{T}^{(1)} \,|\, \vec{p}_1, \vec{p}_2 \rangle$$

$$= \langle \vec{p}_1+\vec{Q}, \vec{p}_2 - \vec{Q} \,|\, \frac{1}{2L^3} \sum_{\vec{k}_1 \vec{k}_2 \vec{q}} V(\vec{q}) \, a^+_{\vec{k}_1+\vec{q}} a^+_{\vec{k}_2-\vec{q}} a_{\vec{k}_2} a_{\vec{k}_1} \,|\, \vec{p}_1, \vec{p}_2 \rangle$$

$$= \frac{1}{2L^3} \sum_{\vec{k}_1 \vec{k}_2 \vec{q}} \langle 0 | a_{\vec{p}_2-\vec{Q}} \, a_{\vec{p}_1+\vec{Q}} \, V(\vec{q}) \, a^+_{\vec{k}_1+\vec{q}} a^+_{\vec{k}_2-\vec{q}} a_{\vec{k}_2} a_{\vec{k}_1} \, a^+_{\vec{p}_1} a^+_{\vec{p}_2} |0\rangle$$

$$= \frac{1}{2L^3} \sum_{\vec{k}_1 \vec{k}_2 \vec{q}} V(\vec{q}) \langle 0 | a_{\vec{p}_2-\vec{Q}} \, a_{\vec{p}_1+\vec{Q}} \, a^+_{\vec{k}_1+\vec{q}} a^+_{\vec{k}_2-\vec{q}} a_{\vec{k}_2} a_{\vec{k}_1} \, a^+_{\vec{p}_1} a^+_{\vec{p}_2} |0\rangle$$

We will finish the evaluation of the amplitude on Tuesday, 02.07.23