The zero particle Hilbert space $F_0^\pm$ is spanned by $|0\rangle$ both for fermions and bosons and is annihilated by $\hat{a}_{\lambda_i}$. There is no upper limit for the number of bosons. On the contrary, if the single particle Hilbert space F_1^- has dimension M $\Rightarrow$ $\hat{a}^+_\lambda F_M^- = 0$ since $\hat{a}^{+2}_\lambda = 0$.

5.4 Occupation number operator

The occupation number operator of the single particle state λ_i is defined as

$$\hat{n}_{\lambda_i} = \hat{a}^+_{\lambda_i} \hat{a}_{\lambda_i} \qquad (5.15)$$

and it fulfills the equation $\hat{n}_{\lambda_i} (\hat{a}^+_{\lambda_i})^{n_{\lambda_i}} |0\rangle = n_{\lambda_i} (\hat{a}^+_{\lambda_i})^{n_{\lambda_i}} |0\rangle$.

Thus, $(\hat{a}^+_{\lambda_i})^{n_{\lambda_i}} |0\rangle$ is an eigenstate of $\hat{n}_{\lambda_i}$ with eigenvalue n_{λ_i}. More generally:

$$\hat{n}_{\lambda_i} \prod_j (\hat{a}^+_{\lambda_j})^{n_{\lambda_j}} |0\rangle = n_{\lambda_i} \prod_j (a^+_{\lambda_j})^{n_{\lambda_j}} |0\rangle \qquad (5.16)$$

as can be proven using commutation relations. Since $[\hat{n}_{\lambda_i}, \hat{n}_{\lambda_j}] = 0$ one sees that $\{\hat{n}_{\lambda_i}\}$ represents a complete set of operators for any Hilbert space $F_N^\pm$ and justifies the validity of the occupation number representation $|\psi\rangle_\pm = |\{n_{\lambda_i}\}\rangle$ already given in (5.10).

5.5 Representation of operators in I and II quantization

In II Q. every operator can be written in terms of creation and annihilation operators. In particular one can distinguish between one-body operators, two-body operators, mixed operators in which different type of particles interact.

Proof of (5.16)

$$\hat n_{\lambda_i} \prod_j \left(\hat a^+_{\lambda_j}\right)^{n_{\lambda_j}} |0\rangle = \prod_{j<i} \left(\hat a^+_{\lambda_j}\right)^{n_{\lambda_j}} \hat n_{\lambda_i} \left(\hat a^+_{\lambda_i}\right)^{n_{\lambda_i}} \prod_{j>i} \left(\hat a^+_{\lambda_j}\right)^{n_{\lambda_j}} |0\rangle =$$

$$= \prod_{j<i} \hat a^{+\,n_{\lambda_j}}_{\lambda_j} \left(a^+_{\lambda_i} (\pm 1)^{n_{\lambda_i}} \hat a^{+\,n_{\lambda_i}}_{\lambda_i} \hat a_{\lambda_i} + n_{\lambda_i} \hat a^{+\,n_{\lambda_i}-1}_{\lambda_i} \right) \prod_{j>i} \hat a^{+\,n_{\lambda_j}}_{\lambda_j} |0\rangle =$$

$$= \pm \prod_{j<i} \hat a^{+\,n_{\lambda_j}}_{\lambda_j} \hat a^{+\,n_{\lambda_i}+1}_{\lambda_i} \prod_{j>i} \hat a^{+\,n_{\lambda_j}}_{\lambda_j} (\pm 1)^{\sum_{j>i} n_{\lambda_j}} \hat a_{\lambda_i} |0\rangle +$$

$$+ n_{\lambda_i} \prod_j \hat a^{+\,n_{\lambda_j}}_{\lambda_j} |0\rangle \qquad \text{q.e.d.}$$

The first equality follows from $[a_{\lambda_i}, a^+_{\lambda_j}]_\pm = \delta_{\lambda_i \lambda_j}$ and $[a_{\lambda_i}, a_{\lambda_j}]_\pm = 0$ which directly implies $[\hat n_{\lambda_i}, a^+_{\lambda_j}] = 0$ if $\lambda_i \neq \lambda_j$ both for fermions and bosons. The second equality relies on the relation

$$a_\lambda \, a^{+\,n_\lambda}_\lambda = (\pm 1)^{n_\lambda} a^{+\,n_\lambda}_\lambda a_\lambda + n_\lambda a^{+\,n_\lambda - 1}_\lambda$$

which holds both for fermions and bosons (with the different signs)

- fermions: $n = 0$ trivial
  $n = 1$ $[a_\lambda, a^+_\lambda]_+ = 1$ is the canonical anticom. relation
- bosons the relation can be rewritten as $[a_\lambda, a^{+\,n}_\lambda] = n\, a^{+\,n-1}_\lambda$
  $n = 0$ trivial as $[a_\lambda, 1] = 0$
  $n-1$ assume to hold

$$[a_\lambda, a^{+\,n}_\lambda] = a^+_\lambda [a, a^{+\,n-1}_\lambda] + [a_\lambda, a^+_\lambda]\, a^{+\,n-1}_\lambda =$$

$$a^+_\lambda (n-1) a^{+\,n-2}_\lambda + a^{+\,n-1}_\lambda = n\, a^{+\,n-1}_\lambda \qquad \text{q.e.d.}$$

One body operators

One body operators $\hat{O}_1$ acting on the N-particle Hilbert space $F_N^{\pm}$ are defined as:

$$\hat{O}_{\mathbf{1}} = \sum_{j=1}^{N} \hat{o}_j \tag{5.17}$$

with $\hat{o}_j$ an ordinary operator acting on particle j, as for example

- Kinetic operator $\quad \hat{T} = \sum_{j=1}^{N} \frac{\hat{p}_j^2}{2m} = -\sum_{j=1}^{N} \frac{\hbar^2 \nabla_j^2}{2m} = \sum_{j=1}^{N} \hat{t}_j$
- External potential operator $\quad \hat{V} = \sum_{j=1}^{N} v(\hat{\vec{r}}_j) = \sum_{j=1}^{N} \hat{v}_j$
- Spin operator $\quad \hat{\vec{S}} = \sum_{j=1}^{N} \frac{\hbar}{2} \vec{\sigma}_j = \sum_{j=1}^{N} \hat{s}_j$

In general, in IQ. one writes $\hat{O} = \sum_{\lambda_1\lambda_2} o_{\lambda_1\lambda_2} |\lambda_1\rangle\langle\lambda_2|$, where $o_{\lambda_1\lambda_2} = \langle\lambda_1|\hat{O}|\lambda_2\rangle$ are the matrix element of the operator $\hat{o}$ on the complete basis $|\lambda\rangle$.

Let us consider first a 1-body operator that is diagonal in the basis $|\lambda\rangle$ i.e. $\quad \hat{o} = \sum_{\lambda} o_\lambda |\lambda\rangle\langle\lambda|$.

We introduce now, for convenience, the notation

$$|\nu_1, \dots, \nu_N\rangle_{\pm} \equiv \hat{S}_{\pm} \bigotimes_{j=1} |\nu_j\rangle \tag{5.18}$$

We now calculate the action of the one-body operator on a symmetrized state

$$\hat{O}_1 |\nu_1, \dots, \nu_N\rangle_{\pm} = \sum_{j,\lambda} o_\lambda |\lambda\rangle_j\langle\lambda| \mathcal{N} \sum_{P} \bigotimes_{j'=1}^{N} |\nu_{p(j')}\rangle [\mathrm{sign}(p)]^{2s} = \quad \begin{matrix}\langle\lambda| \text{ acts on the} \\ j\text{th particle}\end{matrix}$$

$$= \sum_{j,\lambda} o_\lambda \mathcal{N} \sum_{P} \delta_{\lambda \nu_{p(j)}} \bigotimes_{j'=1}^{N} |\nu_{p(j')}\rangle [\mathrm{sign}(p)]^{2s} = \quad \text{relabelling } \sum_j$$

$$= \sum_{j,\lambda} o_\lambda \delta_{\lambda\nu_j} |\nu_1,\dots,\nu_N\rangle_\pm = \sum_\lambda o_\lambda n_\lambda |\nu_1,\dots,\nu_N\rangle_\pm \qquad (5.18)$$

where n_λ counts how many times the quantum number λ appears in the set $\{\nu_j\}$. Finally we can use (5.16) to conclude that (5.18) becomes:

$$\hat{O}_1 |\nu_1,\dots,\nu_N\rangle_\pm = \sum_\lambda o_\lambda \hat{a}^+_\lambda \hat{a}_\lambda |\nu_1,\dots,\nu_N\rangle_\pm \qquad (5.19)$$

The last step to a generic formulation of the one-body operator is the change of basis

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

$$\Updownarrow$$

$$\hat{a}^+_\lambda = \sum_\mu \langle\mu|\lambda\rangle \hat{a}^+_\mu \quad \Leftrightarrow \quad \hat{a}_\lambda = \sum_\mu \langle\lambda|\mu\rangle \hat{a}_\mu \qquad (5.20)$$

Consequently:

$$\hat{O}_1 = \sum_\lambda \langle\lambda|O|\lambda\rangle \hat{a}^+_\lambda \hat{a}_\lambda = \sum_{\mu\nu\lambda} \hat{a}^+_\mu \underbrace{\langle\mu|\lambda\rangle\langle\lambda|O|\lambda\rangle\langle\lambda|\nu\rangle}_{o_{\mu\mu'}} \hat{a}_\nu$$

$$\hat{O}_1 = \sum_{\mu\nu} \hat{a}^+_\mu \langle\mu|\hat{O}|\nu\rangle \hat{a}_\nu \qquad (5.21)$$

1-body operators in <u>II quantization</u> are composed of <u>products</u> of creation and annihilation operators, weighted by the appropriate <u>matrix element</u> of the operator calculated in <u>I quantization</u>

Examples of 1-body operators

- Kinetic energy in position-spin representation

$$\hat{T} = \sum_{\mu\nu} \hat{a}^+_\mu \langle\mu|\hat{t}|\nu\rangle \hat{a}_\mu = \sum_{\mu\nu} \hat{a}^+_\mu \sum_{\sigma\sigma'} \int d\vec{r} d\vec{r}' \langle\mu|\vec{r}\sigma\rangle\langle\vec{r}\sigma|\hat{t}|\vec{r}'\sigma'\rangle\langle\vec{r}'\sigma'|\nu\rangle \hat{a}_\nu$$

$$= \sum_\sigma \int d\vec{r} \underbrace{\left(\sum_\mu \hat{a}^+_\mu \varphi^*_\mu(\vec{r}\sigma)\right)}\left(-\frac{\hbar^2}{2m}\nabla^2_{\vec{r}}\right)\underbrace{\left(\sum_\nu \hat{a}_\nu \varphi_\nu(\vec{r}\sigma)\right)}$$

$$= \sum_\sigma \int d\vec{r} \quad \hat{\psi}^+_\sigma(\vec{r}) \left(-\frac{\hbar^2}{2m}\nabla^2_{\vec{r}}\right) \hat{\psi}_\sigma(\vec{r}) \tag{5.22}$$

where we have introduced the field operator $\hat{\psi}_\sigma(\vec{r}) \equiv \sum_\nu \hat{a}_\nu \varphi_\nu(\vec{r}\sigma)$

- Kinetic energy in momentum representation

$$\hat{T} = \sum_{\vec{k}\sigma} a^+_{\vec{k}\sigma} \langle\vec{k}\sigma|\hat{t}|\vec{k}\sigma\rangle a_{\vec{k}\sigma} = \sum_{\vec{k}\sigma} \frac{1}{V}\int d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}}\left(-\frac{\hbar^2\nabla^2}{2m}\right)e^{i\vec{k}\cdot\vec{r}} =$$

$$= \sum_{\vec{k}\sigma} \hat{n}_{\vec{k}\sigma} \frac{\hbar^2 k^2}{2m} . \tag{5.23}$$

- density operator in position representation

$$\hat{\rho}(\vec{r}) = \sum_i \delta(\vec{r}-\hat{r}_i) = \sum_{\mu\nu} \hat{a}^+_\mu \langle\mu|\delta(\vec{r}-\hat{r})|\nu\rangle \hat{a}_\nu =$$

$$= \sum_\sigma \int d\vec{s}\; \hat{a}^+_\mu \langle\mu|\vec{s}\sigma\rangle \delta(\vec{r}-\vec{s}) \langle\vec{s}\sigma|\nu\rangle \hat{a}_\nu =$$

$$\sum_\sigma \psi^+_\sigma(\vec{r})\psi_\sigma(\vec{r}) . \tag{5.24}$$

- density operator in momentum representation

$$\hat{\rho}(\vec{r}) = \sum_\sigma \sum_{\vec{k}\vec{k}'} \hat{a}^+_{\vec{k}\sigma}\langle\vec{k}\sigma|\delta(\vec{r}-\hat{r})|\vec{k}'\sigma\rangle \hat{a}_{\vec{k}'\sigma} =$$

$$= \sum_{\substack{\sigma\\ \vec{k}\vec{k}'}} \frac{1}{V}\int d\vec{s}\; \hat{a}^+_{\vec{k}\sigma} e^{-i(\vec{k}-\vec{k}')\cdot\vec{s}} \delta(\vec{r}-\vec{s})\, \hat{a}_{\vec{k}'\sigma}$$

$$= \sum_{\vec{k}\vec{k}'\sigma} \frac{1}{V} \hat{a}^+_{\vec{k}\sigma} a_{\vec{k}'\sigma} e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}} = \frac{1}{V}\sum_{\vec{k}\vec{q}\sigma} e^{i\vec{q}\cdot\vec{r}} \hat{a}^+_{\vec{k}\sigma}\hat{a}_{\vec{k}+\vec{q}\sigma} \tag{5.25}$$

• particle current density operator

This operator is related to the particle density operator by the continuity equation

$$\partial_t \hat{\rho} + \vec{\nabla}\cdot\hat{\vec{J}} = 0$$

To find its form, valid also in presence of a finite vector potential $\vec{A}$, we notice that, in analytical mechanics, small variations δH of the Hamilton function H due to variations $\delta\vec{A}$ in the vector potential are related to $\vec{J}$ by:

$$\delta H = -q\int d\vec{r}\, \vec{J}\cdot\delta\vec{A}$$

We use this expression with $\hat{H}$ given by the kinetic operator $\hat{T}_A$:

$$\hat{H} = \hat{T}_A = \frac{1}{2m}\sum_\sigma \int d\vec{r}\, \hat{\psi}^+_\sigma(\vec{r})\left[\frac{\hbar}{i}\vec{\nabla}_r - q\vec{A}\right]^2 \hat{\psi}_\sigma(\vec{r})$$

$$= \hat{T} + \sum_\sigma \int d\vec{r}\left[-\hat{\psi}^+_\sigma(\vec{r})\frac{q\hbar}{2mi}\left(\vec{\nabla}\cdot\vec{A} + \vec{A}\cdot\vec{\nabla}\right)\hat{\psi}_\sigma(\vec{r})\right]$$

$$+ \frac{q^2}{2m}A^2\,\hat{\psi}^+_\sigma(\vec{r})\hat{\psi}_\sigma(\vec{r}).$$

Notice that there is one term where $\vec{\nabla}$ acts on $\vec{A}$. By partial integration this is shifted to $\hat{\psi}^+_\sigma(\vec{r})$:

$$\hat{H} = \hat{T} + \sum_\sigma\int d\vec{r}\, \frac{q\hbar}{2mi}\left[\vec{A}\cdot\left[\left(\vec{\nabla}\psi^+_\sigma(\vec{r})\right)\hat{\psi}_\sigma(\vec{r}) - \psi^+_\sigma(\vec{r})\left(\vec{\nabla}\psi_\sigma(\vec{r})\right)\right]\right.$$

$$\left. + \frac{q^2}{2m}A^2\hat{\rho}_\sigma(\vec{r})\right\}$$

The variation of $\vec{A}$ can now be easily performed since:

$$\hat{H} = \hat{T} - q\sum_\sigma d\vec{r}\,\vec{A}\cdot\hat{\vec{J}}_\sigma$$

where $\hat{\vec{J}}_\sigma(\vec{r}) = \hat{\vec{J}}_\sigma^{\,para} + \hat{\vec{J}}_\sigma^{\,dia}$ = paramagnetic + diamagnetic and

$$\begin{cases} \hat{\vec{J}}_\sigma^{\,para}(\vec{r}) = \dfrac{\hbar}{2mi}\left[\hat{\psi}_\sigma^+(\vec{r})\,\vec{\nabla}\,\hat{\psi}_\sigma(\vec{r}) - \left(\vec{\nabla}\,\hat{\psi}_\sigma^+(\vec{r})\right)\hat{\psi}_\sigma(\vec{r})\right] \\ \hat{\vec{J}}_\sigma^{\,dia}(\vec{r}) = -\dfrac{q}{m}\,\vec{A}\,\hat{\rho}_\sigma(\vec{r}) \end{cases} \tag{5.26}$$

In momentum representation

$$\begin{cases} \vec{J}_\sigma^{\,para}(\vec{r}) = \dfrac{\hbar}{mV}\sum\limits_{\vec{k}\vec{q}}\left(\vec{k}+\dfrac{\vec{q}}{2}\right)e^{i\vec{q}\cdot\vec{r}}\,\hat{a}^+_{\vec{k}\sigma}\,\hat{a}_{\vec{k}+\vec{q}\sigma} \\ \vec{J}_\sigma^{\,dia}(\vec{r}) = -\dfrac{q}{mV}\,\vec{A}(\vec{r})\sum\limits_{\vec{k}\vec{q}} e^{i\vec{q}\cdot\vec{r}}\,\hat{a}^+_{\vec{k}\sigma}\,\hat{a}_{\vec{k}+\vec{q}\sigma} \end{cases} \tag{5.27}$$

Finally, in first quantization:

$$\hat{j}(\vec{r},t) = \frac{1}{2m}\sum_{i=1}^{N}\left[\left(\hat{\vec{p}}_i - q\vec{A}(\hat{\vec{r}}_i,t)\right)\delta(\vec{r}-\hat{\vec{r}}_i) + \delta(\vec{r}-\hat{\vec{r}}_i)\left(\hat{\vec{p}}_i - q\vec{A}(\hat{\vec{r}}_i,t)\right)\right]$$

- <u>spin operator</u> for spin ½ fermions in position representation

$$\hat{\vec{S}} = \sum_{\mu\nu}{}' \hat{a}^+_\mu \langle\mu|\hat{\vec{s}}|\nu\rangle a_\nu .$$ If we take $|\nu\rangle = |\vec{r}\tau\rangle$ and $\tau = \pm\frac{1}{2}$

for spin ½ fermions:

$\hat{s}_\alpha = \frac{\hbar}{2}\sigma_\alpha$ in the basis $\uparrow,\downarrow$ where $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

are the Pauli matrices. We thus obtain

$$\begin{cases} \hat{S}_x = \dfrac{\hbar}{2}\displaystyle\int d\vec{r}\ \psi^+_\uparrow(\vec{r})\psi_\downarrow(\vec{r}) + \psi^+_\downarrow(\vec{r})\psi_\uparrow(\vec{r}) \\ \hat{S}_y = -\dfrac{i\hbar}{2}\displaystyle\int d\vec{r}\ \psi^+_\uparrow(\vec{r})\psi_\downarrow(\vec{r}) - \psi^+_\downarrow(\vec{r})\psi_\uparrow(\vec{r}) \\ \hat{S}_z = \dfrac{\hbar}{2}\displaystyle\int d\vec{r}\ \psi^+_\uparrow(\vec{r})\psi_\uparrow(\vec{r}) - \psi^+_\downarrow(\vec{r})\psi_\downarrow(\vec{r}) \end{cases} \tag{5.28}$$

In momentum representation $$\hat{\vec{S}} = \sum_{\vec{k}\tau\tau'} \hat{a}^+_{\vec{k}\tau}\,\vec{\sigma}_{\tau\tau'}\,a_{\vec{k}\tau'} . \tag{5.29}$$

Two-body operator in II quantization

A two-body operator in a N-particle system is defined in I quantization as

$$\hat{O}_2 = \frac{1}{2} \sum_{j,\, k \neq j} \hat{o}_{jk} \tag{5.30}$$

Only 2 particles are involved in the interaction, thus the operator $\hat{O}_2$ can be characterized in terms of his action on two-particle states.

$$o_{\lambda\mu\mu'\lambda'} \equiv \underbrace{\left(\langle\lambda| \otimes \langle\mu|\right)}_{\text{NOT}}\hat{o}\underbrace{\left(|\mu'\rangle \otimes |\lambda'\rangle\right)}_{\text{SYMMETRIZED!}}$$

Notice: $\left(|\mu\rangle \otimes |\lambda\rangle\right)^{+} = \left(\langle\lambda| \otimes \langle\mu|\right)$

We assume to start with the two-body operator to be diagonal in the unfactrized basis: $\hat{o} = \sum_{\lambda\mu} o_{\lambda\mu}\left(|\mu\rangle \otimes |\lambda\rangle\right)\left(\langle\lambda| \otimes \langle\mu|\right)$. It follows that, when applied to the generic symmetrized/antisymmetrized state

$$\hat{O}_2 |\nu_1, \dots, \nu_N\rangle = \frac{1}{2} \sum_{\substack{j\, k\neq j \\ \lambda\mu}} o_{\lambda\mu} \left(|\mu\rangle_j \otimes |\lambda\rangle_k\right)\left({}_k\langle\lambda| \otimes {}_j\langle\mu|\right) \sum_{p \in S_N} \bigotimes_{j'=1}^{N} |\nu_{p(j')}\rangle \left[\mathrm{sign}(p)\right]^{2S}$$

$$= \frac{1}{2} \sum_{\substack{j\, k\neq j \\ \lambda\mu}} o_{\lambda\mu} \sum_{p \in S_N} \delta_{\mu \nu_{p(j)}} \delta_{\lambda \nu_{p(k)}} \bigotimes_{j'=1}^{N} |\nu_{p(j')}\rangle \left[\mathrm{sign}(p)\right]^{2S} =$$

$j \neq k \Rightarrow p(j) \neq p(k)$

$$= \frac{1}{2} \sum_{\substack{j\, k\neq j \\ \lambda\mu}} o_{\lambda\mu} \delta_{\mu\nu_j} \delta_{\lambda\nu_k} |\nu_1, \dots, \nu_N\rangle = \frac{1}{2} \sum_{\lambda\mu} o_{\lambda\mu} n_\mu \left(n_\lambda - \delta_{\lambda\mu}\right) |\nu_1, \dots, \nu_N\rangle$$

if $\lambda = \mu$ the sum over k will give necessarily $n_\lambda - 1$

$$= \frac{1}{2} \sum_{\lambda\mu} o_{\lambda\mu} \hat{n}_\mu \left(\hat{n}_\lambda - \delta_{\lambda\mu}\right) |\nu_1, \dots, \nu_N\rangle = \frac{1}{2} \sum_{\lambda\mu} o_{\lambda\mu}\left(\hat{a}^{+}_\mu \hat{a}_\mu \hat{a}^{+}_\lambda \hat{a}_\lambda - \delta_{\lambda\mu} \hat{a}^{+}_\mu \hat{a}_\mu\right) |\nu_1, \dots, \nu_N\rangle$$

$$= \frac{1}{2} \sum_{\lambda\mu} o_{\lambda\mu} \hat{a}^{+}_\mu \hat{a}^{+}_\lambda \hat{a}_\lambda \hat{a}_\mu |\nu_1, \dots, \nu_N\rangle \tag{5.31}$$

Where in the last equality we have used the commutation relations:

$$a^+_\mu a_\mu a^+_\lambda a_\lambda = a^+_\mu (\delta_{\mu\lambda} \mp a^+_\lambda a_\mu) a_\lambda = a^+_\mu a_\mu \delta_{\lambda\mu} + a^+_\mu a^+_\lambda a_\lambda$$

The general result is obtained via the change of basis (5.20) which yields:

$$\boxed{\hat{O}_2 = \frac{1}{2} \sum_{\substack{\lambda\mu \\ \lambda'\mu'}}' \hat{a}^+_\lambda \hat{a}^+_\mu \underbrace{(\langle\lambda| \otimes \langle\mu|) \hat{o} (|\mu'\rangle \otimes |\lambda'\rangle)}_{\equiv\, O_{\lambda\mu\mu'\lambda'}} \hat{a}_{\mu'} \hat{a}_{\lambda'} \qquad (5.32)}$$

2-body operators in II quantization are composed of products of 2 creation and 2 annihilation operators, weighted by the appropriate matrix element of the operator calculated in I quantization.

A classical example of 2-body operator is given by the Coulomb interaction

$$\hat{V}_{ee} = \frac{1}{2} \sum_{j,k\neq j}^{N} \hat{v}_{ee,jk} = \frac{1}{2} \sum_{j,k\neq j}^{N} v_{ee}(\hat{\vec{r}}_j - \hat{\vec{r}}_k)$$

If we introduce the single particle basis $|\vec{r}\sigma\rangle$ and take into account that:

$$\left(\langle\vec{r}_1\sigma_1| \otimes \langle\vec{r}_2\sigma_2|\right) v_{ee}(\hat{\vec{r}}_1 - \hat{\vec{r}}_2) \left(|\vec{r}_3\sigma_3\rangle \otimes |\vec{r}_4\sigma_4\rangle\right)$$

$$= \delta(\vec{r}_1 - \vec{r}_4)\, \delta(\vec{r}_2 - \vec{r}_3)\, v_{ee}(\vec{r}_1 - \vec{r}_2)\, \delta_{\sigma_1\sigma_4} \delta_{\sigma_2\sigma_3}$$

we obtain

$$\hat{V}_{ee} = \frac{1}{2} \int d\vec{r}_1 d\vec{r}_2 \sum_{\sigma_1\sigma_2} \psi^+_{\sigma_1}(\vec{r}_1)\, \psi^+_{\sigma_2}(\vec{r}_2)\, v_{ee}(\vec{r}_1 - \vec{r}_2)\, \psi_{\sigma_2}(\vec{r}_2)\, \psi_{\sigma_1}(\vec{r}_1) \qquad (5.33)$$

In the momentum representation

$$\hat{V}_{ee} = \frac{1}{2}\int d\vec{r}_1 d\vec{r}_2 \sum_{\sigma_1\sigma_2} \frac{1}{V^2} \sum_{\vec{k}_1\vec{k}_2\vec{k}_3\vec{k}_4} e^{-i(\vec{k}_1\vec{r}_1 + \vec{k}_2\vec{r}_2 - \vec{k}_3\vec{r}_2 - \vec{k}_4\vec{r}_1)} \hat{a}^+_{\vec{k}_1\sigma_1}\hat{a}^+_{\vec{k}_2\sigma_2}\hat{a}_{\vec{k}_3\sigma_2}\hat{a}_{\vec{k}_4\sigma_1}$$

$$\times v(\vec{r}_1-\vec{r}_2) = \left(\begin{array}{ll} \vec{k}=\vec{k}_4 & \sigma=\sigma_1 \\ \vec{k}'=\vec{k}_3 & \sigma'=\sigma_2 \\ \vec{q}=\vec{k}_3-\vec{k}_2 = \vec{k}_4-\vec{k}_1 & \end{array}\right) \text{ and } \frac{1}{V}\sum_{\vec{k}} e^{i\vec{r}\cdot\vec{k}} = \delta(\vec{r})$$

$$= \frac{1}{2V}\sum_{\vec{q}}\sum_{\vec{k}\vec{k}'}\sum_{\sigma\sigma'} \hat{a}^+_{\vec{k}+\vec{q}\sigma}\hat{a}^+_{\vec{k}'-\vec{q}\sigma'}\hat{a}_{\vec{k}'\sigma'}\hat{a}_{\vec{k}\sigma}\,\tilde{v}_{ee}(\vec{q}) \qquad (5.34)$$

where $\tilde{v}_{ee}(\vec{q}) = \int d\vec{r}\, e^{i\vec{q}\cdot\vec{r}} \frac{e^2}{4\pi\varepsilon_0 r} = \lim_{\eta\to 0}\int d\vec{r}\, e^{i\vec{q}\cdot\vec{r}-\eta r}\frac{e^2}{4\pi\varepsilon_0 r} = \frac{e^2}{q^2\varepsilon_0}$

<u>Spin interaction Hamiltonian</u> as a representation of the Coulomb interaction on a reduced single particle basis (effective Hamiltonian)

$$\hat{H}_{Heis} = \frac{1}{2}\sum_{i,j\neq i} J_{ij}\hat{S}_i\cdot\hat{S}_j = \frac{1}{2}\sum_{i,j\neq i} J_{ij}\sum_{\substack{\alpha\tau\tau'\\ \rho\rho'}} \hat{a}^+_{i\tau}\hat{a}_{i\tau'}\hat{a}^+_{j\rho}a_{j\rho'}\sigma^\alpha_{\tau\tau'}\sigma^\alpha_{\rho\rho'}$$

where $\hat{S}_i$ is the spin operator for the (valence electrons on the) atom i.

- Mixed operators. As an example of mixed operator we take the one describing the interaction of <u>electrons and phonons.</u>

The electron-ion interaction as we introduced it in the Hamiltonian for the solid (1.1) reads:

$$\hat{V}_{ei} = -\sum_{j\alpha}\frac{Z_\alpha e^2}{4\pi\varepsilon_0}\frac{1}{|\hat{\vec{r}}_j-\hat{\vec{R}}_\alpha|} = \sum_\alpha \int d\vec{r}\, \overbrace{\sum_j \delta(\vec{r}-\hat{\vec{r}}_j)}^{\hat{\rho}_{el}(\vec{r})} \left(-\frac{Z_\alpha e^2}{4\pi\varepsilon_0}\right)\frac{1}{|\vec{r}-\hat{\vec{R}}_\alpha|}$$

where, to underline their operatorial nature we have explicitly added an hat to $\vec{r}_j$ and $\vec{R}_\alpha$, and, in the second equality, we have explicitly introduced the electron density operator

If we now consider that $\hat{\vec{R}}_\alpha = \vec{R}^0_\alpha + \hat{\vec{u}}_\alpha$ and that $\vec{u}_\alpha$, the displacement is the only (small) dynamical part:

$$\hat{V}_{ei} = \hat{V}_{ei}^{static} + \hat{V}_{el-ph}$$

dealt with for the Bloch electrons

By expanding to first order in the displacement $\vec{u}_\alpha$ we obtain:

$$\hat{V}_{el-ph} = - \int d\vec{r}\ \hat{\rho}_{el}(\vec{r}) \sum_{\alpha\tau} \hat{\vec{u}}_{\alpha\tau} \cdot \vec{\nabla}_{\vec{r}}\, v_{at}(\vec{r} - \vec{R}^0_{\alpha\tau}) \tag{5.35}$$

where, according to (3.38) and (3.31)

$$\hat{\vec{u}}_{\alpha\tau} = \frac{1}{\sqrt{N_{cell} M_\tau}} \sum_{\vec{q}j} \sqrt{\frac{\hbar}{2\omega_j(\vec{q})}}\ \vec{e}_\tau(\vec{q},j) \left(\hat{b}_{\vec{q},j} + \hat{b}^+_{-\vec{q},j} \right) e^{i\vec{q}\cdot\vec{R}^0_\alpha}$$

It is more convenient to write the el-ph interaction in momentum space

$$v_{at}(\vec{r}) = \frac{1}{V} \sum_{\vec{p}} \tilde{v}_{at}(\vec{p})\, e^{i\vec{p}\cdot\vec{r}} \Rightarrow \vec{\nabla}_{\vec{r}} v_{at}(\vec{r}) = \frac{i}{V} \sum_{\vec{p}} \vec{p}\ \tilde{v}_{at}(\vec{p})\, e^{i\vec{p}\cdot\vec{r}}$$

where $\vec{p}$ is fixed only by the boundary condition of the crystal: $\Rightarrow$
$\vec{p} = \vec{q} + \vec{G}$ where $\vec{q} \in 1BZ$ and $\vec{G} \in RL$

$$\vec{\nabla}_{\vec{r}} v_{at}(\vec{r} - \vec{R}^0_\alpha) = \frac{i}{V} \sum_{\vec{q}} \sum_{\vec{G}} (\vec{q}+\vec{G})\ \tilde{v}_{at}(\vec{q}+\vec{G})\ e^{i(\vec{q}+\vec{G})\cdot(\vec{r} - \vec{R}^0_\alpha)}$$

Since $\vec{G}\cdot\vec{R}^0_\alpha = 2\pi n$

$$\vec{\nabla}_{\vec{r}} v_{at}(\vec{r} - \vec{R}^0_\alpha) = \frac{i}{V} \sum_{\vec{q}\in 1BZ} \sum_{\vec{G}\in RL} (\vec{q}+\vec{G})\ \tilde{v}_{at}(\vec{q}+\vec{G})\ e^{i(\vec{q}+\vec{G})\cdot\vec{r} - i\vec{q}\cdot\vec{R}^0_\alpha}$$

Finally we also write the electron density in momentum representation (5.25) and obtain:

$$\hat{V}_{el-ph} = -\int d\vec{r} \sum_{\alpha\tau} \frac{1}{V} \sum_{\vec{k}_1\vec{k}_2\sigma} e^{i\vec{k}_2\vec{r}}\, \hat{a}^+_{\vec{k}_1\sigma}\, \hat{a}_{\vec{k}_1+\vec{k}_2\sigma} \cdot$$

$$\frac{1}{\sqrt{N_{cell} M_\tau}} \sum_{\vec{q}_1 j} \sqrt{\frac{\hbar}{2\omega_j(\vec{q}_1)}}\, \vec{e}_\tau(\vec{q}_1, j) \left(\hat{b}_{\vec{q}_1 j} - \hat{b}^+_{-\vec{q}_1, j}\right) e^{i\vec{q}_1 \cdot \vec{R}^0_\alpha}$$

$$\frac{i}{V} \sum_{\vec{q}_2 \in 1BZ} \sum_{\vec{G}\in RL} (\vec{q}_2 + \vec{G})\, \tilde{v}_{at}(\vec{q}_2 + \vec{G})\, e^{i(\vec{q}_2+\vec{G})\cdot\vec{r} - i\vec{q}_2 \cdot \vec{R}^0_\alpha}$$

$$\frac{1}{N_{cell}} \sum_\alpha e^{i(\vec{q}_1 - \vec{q}_2)\vec{R}^0_\alpha} = \delta_{\vec{q}_1,\vec{q}_2} \qquad \frac{1}{V}\int_V d\vec{r}\, e^{i(\vec{k}_2 + \vec{q}_2 + \vec{G})\vec{r}} = \delta_{\vec{k}_2, -\vec{q}_2 - \vec{G}}$$

$$\hat{V}_{el-ph} = -\sum_\tau \sum_{\vec{k}\vec{q}jG} \hat{a}^+_{\vec{k}\sigma}\, \hat{a}_{\vec{k}-\vec{q}-\vec{G}\sigma} \left(\hat{b}_{\vec{q},j} - \hat{b}^+_{-\vec{q},j}\right) \tag{5.36}$$

$$\frac{1}{V}\sqrt{\frac{N_{cell}}{M_\tau}\frac{\hbar}{2\omega_j(\vec{q})}}\; \vec{e}_\tau(\vec{q}, j)\cdot(\vec{q}+\vec{G})\; \tilde{v}_{at}(\vec{q}+\vec{G})$$

where $|\vec{k}| \in [0, +\infty)$ while $\vec{q} \in 1BZ$. The interpretation of (5.36) is the one of a scattering event in which an electron of momentum $\vec{k} - \vec{q} - \vec{G}$ is scattered into one of momentum $\vec{k}$ since either a phonon of momentum $\vec{q}$ is destroyed or one of momentum $-\vec{q}$ is created. One distinguishes

- normal processes $\vec{G} = 0$
- Umklapp process $\vec{G} \neq 0$

The normal processes dominate the picture since $\tilde{v}_{at}(\vec{q}+\vec{G}) \sim \frac{1}{|\vec{q}+\vec{G}|^2}$.

If we assume Bloch electrons we obtain for the density operator:

$$\hat{\rho}_{el}(\vec{r}) = \sum_{\substack{n\vec{k}\sigma \\ n'\vec{k}'\sigma'}} \langle n\vec{k}\sigma | \delta(\vec{r} - \hat{\vec{r}}) | n'\vec{k}'\sigma' \rangle \, a^{+}_{n\vec{k}\sigma} a_{n'\vec{k}'\sigma'}$$

$$= \sum_{\substack{n\vec{k} \\ n'\vec{k}'}} \frac{1}{V} e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}} u^{*}_{n\vec{k}}(\vec{r}) u_{n'\vec{k}'}(\vec{r}) \, a^{+}_{n\vec{k}\sigma} a_{n'\vec{k}'\sigma}$$

$$= \frac{1}{V} \sum_{\substack{nn' \\ \vec{k}\vec{q}}} e^{+i\vec{q}\cdot\vec{r}} u^{*}_{n\vec{k}}(\vec{r}) u_{n'\vec{k}+\vec{q}}(\vec{r}) a^{+}_{n\vec{k}\sigma} a_{n'\vec{k}+\vec{q}\,\sigma}$$

$$\hat{V}_{el\text{-}ph} = -\int_V d\vec{r} \sum_{\alpha\tau} \frac{1}{V} \sum_{\substack{nn' \\ \vec{q}_1\vec{q}_2}} e^{-i\vec{q}_2\cdot\vec{r}} u^{*}_{n\vec{q}_1}(\vec{r}) u_{n'\vec{q}_1+\vec{q}_2}(\vec{r}) \; a^{+}_{n\vec{q}_1\sigma} a_{n'\vec{q}_1+\vec{q}_2\sigma}$$

$$\times \frac{1}{\sqrt{N_{cell} M_\tau}} \sum_{\vec{q}_3 j} \sqrt{\frac{\hbar}{2\omega_j(\vec{q}_3)}} \; \vec{e}_\tau(\vec{q}_3, j) \left(\hat{b}_{\vec{q}_3,j} - \hat{b}^{+}_{-\vec{q}_3,j}\right) e^{i\vec{q}_3\cdot\vec{R}^0_\alpha}$$

$$\frac{i}{V} \sum_{\vec{q}_4} \sum_{\vec{G}\in RL} (\vec{q}_4+\vec{G}) \; \tilde{v}_{at}(\vec{q}_4+\vec{G}) \; e^{i(\vec{q}_4+\vec{G})\cdot\vec{r} - i\vec{q}_4\cdot\vec{R}^0_\alpha}$$

$$= -\int_V d\vec{r} \sum_{\tau} \frac{1}{V} \sum_{\substack{nn' \\ \vec{q}_1\vec{q}_2\vec{q}_3 j\sigma}} e^{-i\vec{q}_2\cdot\vec{r}} u^{*}_{n\vec{q}_1}(\vec{r}) u_{n'\vec{q}_1+\vec{q}_2}(\vec{r}) \; a^{+}_{n\vec{q}_1\sigma} a_{n'\vec{q}_1+\vec{q}_2\sigma}$$

$$\sqrt{\frac{N_{cell}}{M_\tau} \frac{\hbar}{2\omega_j(\vec{q}_3)}} \; \vec{e}_\tau(\vec{q}_3, j)\cdot(\vec{q}_3+\vec{G}) \; \frac{i}{V} \tilde{v}_{at}(\vec{q}_3+\vec{G}) \, e^{i(\vec{q}_3+\vec{G})\cdot\vec{r}} \left(\hat{b}_{\vec{q}_3 j} + \hat{b}^{+}_{-\vec{q}_3}\right.$$

$$\int_V d\vec{r} = \sum_\alpha \int_{V_{cell}} d\vec{r}' \qquad \vec{r}' = \vec{r} + \vec{R}^0_\alpha$$

$$\hat V_{el-ph} = -\sum_{\tau} \frac{1}{N_{cell} V_{cell}} \sum_{\substack{nn' \\ \vec q_1 \vec q_2 \vec q_3 \\ \alpha j \vec G}} \int_{V_{cell}} d\vec r \; e^{-i \vec q_2 \cdot \cancel{(\vec r + \vec R^0_{\alpha})}} u^*_{n\vec q_1}(\vec r)\, u_{n'\vec q_1+\vec q_2}(\vec r)\; a^+_{n\vec q_1 \sigma}\, a_{n'\vec q_1+c}$$

$$\sqrt{\frac{N_{cell}}{M_\tau}\frac{\hbar}{2\omega_j(\vec q_3)}}\; \vec e_\tau(\vec q_3, j)\cdot(\vec q_3+\vec G)\, \frac{i}{V}\, \tilde v_{et}(\vec q_3+\vec G)\; e^{i(\cancel{\vec q_3}+\vec G)\vec r + i \vec q_3 \vec R^0_\alpha}$$

$$q_2 = +q_3$$

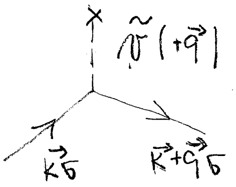
$$= -\sum_{\tau} \frac{1}{V_{cell}} \sum_{\substack{nn' \\ \vec q_1 \vec q_2}} \int_{V_{cell}} d\vec r \; \overbrace{e^{i\vec G\cdot\vec r}\, u^*_{n\vec q_1}(\vec r)\, u_{n'\vec q_1+\vec q_2}(\vec r)}\; a^+_{n\vec q_1\sigma}\, a_{n'\vec q_1+\vec q_2\sigma}$$

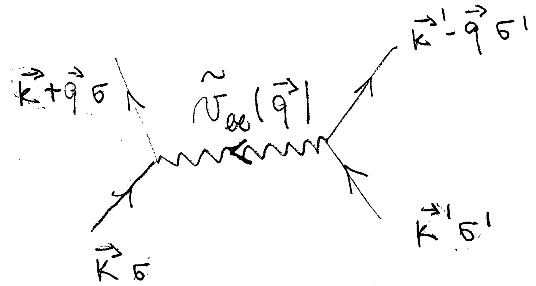
$$\sqrt{\frac{N_{cell}}{M_\tau}\frac{\hbar}{2\omega_j(\vec q_2)}}\; \vec e^{\,*}_\tau(\vec q_2, j)\cdot(\vec G+\vec q_2)\, \frac{i}{V}\, \tilde v_{et}(\vec G+\vec q_2)$$

5.6 Graphical representation of operators in II Q

The operators in II quantization have an appealing representation in terms of Feynmann diagrams.

External potential | **Coulomb interaction**

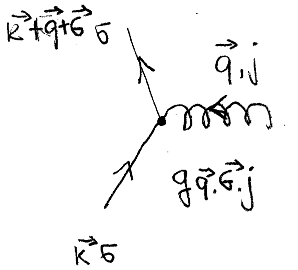


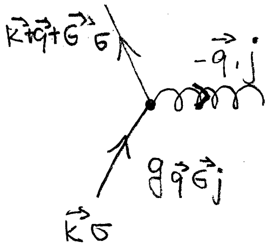


$$\hat{V} = \sum_{\vec{k}\vec{q}\sigma} \tilde{v}(\vec{q})\, \hat{a}^{+}_{\vec{k}+\vec{q}\sigma}\, \hat{a}_{\vec{k}\sigma}$$

$$\hat{V}_{ee} = \frac{1}{2V} \sum_{\vec{q}} \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} \hat{a}^{+}_{\vec{k}+\vec{q}\sigma}\, \hat{a}^{+}_{\vec{k}'-\vec{q}\sigma'}\, \hat{a}_{\vec{k}'\sigma'}\, \hat{a}_{\vec{k}\sigma}$$

Electron-phonon interaction





$$\hat{V}_{el-ph} = \frac{1}{V} \sum_{\vec{k}\vec{q}\vec{G}j} \left(a^{+}_{\vec{k}+\vec{q}+\vec{G}\sigma}\, a_{\vec{k}\sigma}\right)\left(\hat{b}_{\vec{q},j} + \hat{b}^{+}_{-\vec{q}}\right.$$
$$g_{\vec{q}\vec{G}j}$$

where $$g_{\vec{q}\vec{G}j} = \sum_{\tau} \sqrt{\frac{N_{cell}}{M_\tau}\frac{\hbar}{2\omega_j(\vec{q})}}\; \vec{e}_\tau(\vec{q},j)\cdot(\vec{q}+\vec{G})\,\tilde{v}_{at}(\vec{q}+\vec{G})$$