The personal note of the quantum mean field theory for the finite many-body systems

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Contents

Chapter 1

Mean field formalism in the quantum finite many-body system

1.1 The second Quantization

1.1.1 The occupation number picture and the particle-hole picture

Here we first supporse the "Non-interacting fermi system", *i.e.* we suppose the single-particle mean field potential for binding the fermions. For example, the Hartree-Fock potential, Woods-Saxon potential, and so on.

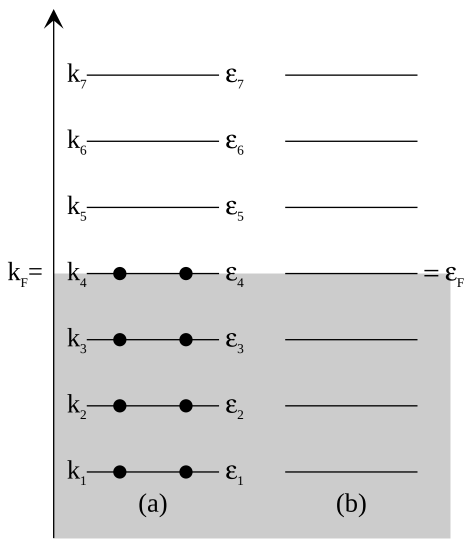


Figure 1.1: (a)the ground state of the occupation number picture. (b)particle-hole picture.

In the quantum mechanics, the ground state in the Non-interacting fermi system can be expressed by the Slater determinant.(N-body wave function in the fermi system.)

$$\Phi_{k_1\dots k_N}(\boldsymbol{r}_1\dots\boldsymbol{r}_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_{k_1}(\boldsymbol{r}_1) & \dots & \phi_{k_1}(\boldsymbol{r}_N) \\ \vdots & \ddots & \vdots \\ \phi_{k_N}(\boldsymbol{r}_1) & \dots & \phi_{k_N}(\boldsymbol{r}_N) \end{vmatrix} \tag{1.1}$$

The Slater determinant is expressed the property of the Pauli principle for each fermions. Now we will introduce the second quantization formula for the occupation number picture. First we define the creation and annihilation operator for fermion by using the anti-commutator relation and the vacuum.

$$\{c_i, c_j^\dagger\} = \delta_{ij} \qquad c_i|-\rangle = 0 \tag{1.2}$$

where $|-\rangle$ is the vacuum, in which no particle exists.

The Slater determinant can be expressed by using these operators as

$$\begin{aligned} \Phi_{k_1\dots k_N}(\boldsymbol{r}_1\dots\boldsymbol{r}_N) &= \frac{1}{\sqrt{N!}}\langle \boldsymbol{r}_1\dots\boldsymbol{r}_N|\prod_{i=1,N} c_{k_i}^\dagger|-\rangle & (1.3) \\ &= \frac{1}{\sqrt{N!}}\langle \boldsymbol{r}_1\dots\boldsymbol{r}_N|1_{k_1},1_{k_2},,,,,1_{k_N}\rangle_a & (1.4) \end{aligned}$$

where $|...\rangle_a$ denotes the anti-symmetrization.

The Slater determinant(the ground state for the Non-interacting fermi system) has the property as

$$c_m|1_{k_1},1_{k_2},,,,,1_{k_N}\rangle = 0 \qquad (m > N) \tag{1.5}$$

By using these operators the fermi vacuum can be defined

$$\left.\begin{array}{ll} a_k|0\rangle & (k > k_F) \\ b_k|0\rangle & (k \leq k_F) \end{array}\right\} = 0$$

Also in the 8-body system(Fig.1.2), *1p-1h states* can be expressed as

$$\begin{aligned} & |1_{k_1\uparrow}, 1_{k_1\downarrow}, , , 1_{k_3\uparrow}, 0_{k_3\downarrow}, 1_{k_4\uparrow}, 1_{k_4\downarrow}, 0, , 1_{k_6\uparrow}, , , , 0\rangle \\ & = c^\dagger_{k_6\uparrow} c_{k_3\downarrow}|0\rangle \\ & = a^\dagger_{k_6\uparrow} b^\dagger_{k_3\downarrow}|0\rangle \\ & = |1^h_{k_3\downarrow} 1^p_{k_6\uparrow}\rangle \end{aligned}$$

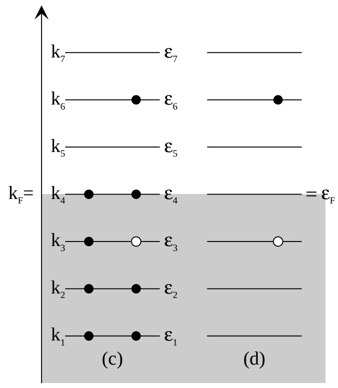


Figure 1.2: (c)*1p-1h* state of the occupation number picture. (d)particle-hole picture.

So the Slater determinant is called "Fermi vacuum". For example, in the 8-body system(Fig.1.1(a)), the Slater determinant(Fermi vacuum) is given by

$$|1_{k_1\uparrow}, 1_{k_1\downarrow}, , , , , 1_{k_4\uparrow}, 1_{k_4\downarrow}\rangle = |1_{k_1\uparrow}, 1_{k_1\downarrow}, , , , , 1_{k_4\uparrow}, 1_{k_4\downarrow}, 0, , , , , , 0\rangle \tag{1.6}$$

$$\equiv |0\rangle \qquad (\textit{'Fermi vacuum'}) \tag{1.7}$$

$$c_{k\sigma}|1_{k_1\uparrow}, 1_{k_1\downarrow}, , , , , 1_{k_4\uparrow}, 1_{k_4\downarrow}, 0, , , , , , 0\rangle = \left\{ \begin{array}{ll} 0 & (k > k_4 = k_F) \\ |1^h_{k\sigma}\rangle & (k \leq k_4 = k_F) \end{array} \right. \tag{1.8}$$

Hence we can define the particle's creation and annihilation operators($a^\dagger, a$) and the hole's creation and annihilation operators($b^\dagger, b$).

$$c_k = \theta(k - k_F)a_k + \theta(k_F - k)b^\dagger_k \tag{1.9}$$

$$c^\dagger_k = \theta(k - k_F)a^\dagger_k + \theta(k_F - k)b_k \tag{1.10}$$

Note that the anti-commutator relation of $a, a^\dagger, b,$ and, $b^\dagger$ can be prooved like that,

$$\begin{aligned} \{c_i, c^\dagger_j\} &= \delta_{ij} \\ &= \{\theta(i - k_F)a_i + \theta(k_F - i)b^\dagger_i, \theta(j - k_F)a^\dagger_j + \theta(k_F - j)b_j\} \\ &= \theta(i - k_F)\theta(j - k_F)\{a_i, a^\dagger_j\} + \theta(k_F - i)\theta(k_F - j)\{b^\dagger_i, b_j\} \\ &\quad +\theta(i - k_F)\theta(k_F - j)\{a_i, b_j\} + \theta(k_F - i)\theta(j - k_F)\{b^\dagger_i, a^\dagger_j\} \end{aligned}$$

when $i = j > k_F(i = j \leq k_F)$, a and $a^\dagger(b$ and $b^\dagger)$ satisfy $\{a_i, a^\dagger_j\} = 1$ ($\{b_i, b^\dagger_j\} = 1$), and also satisfy $\{a_i, a^\dagger_j\} = 0 = \{b_i, b^\dagger_j\}$ when $i \neq j$ because a and $a^\dagger(b$ and $b^\dagger)$ are same kind of fermion. These are self-evident.

$\theta(i - k_F)\theta(k_F - j)$ and $\theta(k_F - i)\theta(j - k_F)$ are vanish when $i = j$ from the step-function's properties, but when $i \neq j$ these terms doesn't vanish. So $\{a_i, b_j\}$ and $\{b^\dagger_i, a^\dagger_j\}$ must be zero when $i \neq j$.

1.1.2 Field Operators in the Coodinate space

By using the single-particle wave function, we can define the creation and annhilation operators in the coordinate space.

$$\psi(\boldsymbol{r}\sigma) = \sum_{k \ni all, s=\uparrow\downarrow} \phi_{ks}(\boldsymbol{r}\sigma)c_{ks} \qquad \psi^\dagger(\boldsymbol{r}\sigma) = \sum_{k \ni all, s=\uparrow\downarrow} \phi^*_{ks}(\boldsymbol{r}\sigma)c^\dagger_{ks} \tag{1.11}$$

With the orthogonality and completeness of the single-particle wave function,

$$\sum_\sigma \int d\boldsymbol{r}\phi^*_{ks}(\boldsymbol{r}\sigma)\phi_{k's'}(\boldsymbol{r}\sigma) = \delta_{ss'}\delta_{kk'} = \langle ks| \left(\sum_\sigma \int d\boldsymbol{r}|\boldsymbol{r}\sigma\rangle\langle\boldsymbol{r}\sigma| \right) |k's'\rangle = \langle ks|k's'\rangle \tag{1.12}$$

$$\sum_{k,s\ni all} \phi_{ks}(\boldsymbol{r}\sigma)\phi^*_{ks}(\boldsymbol{r}'\sigma') = \delta_{\sigma\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}') = \langle \boldsymbol{r}\sigma| \left(\sum_{k,s\ni all} |ks\rangle\langle ks| \right) |\boldsymbol{r}'\sigma'\rangle \quad (1.13)$$

$$\text{where} \quad \phi_{ks}(\boldsymbol{r}\sigma) = \langle \boldsymbol{r}\sigma|ks\rangle \quad (1.14)$$

we can get the anti-commutator relation

$$\left\{\psi(\boldsymbol{r}\sigma), \psi^\dagger(\boldsymbol{r}'\sigma')\right\} = \sum_{k,s\ni all}\sum_{k',s'\ni all} \phi_{ks}(\boldsymbol{r}\sigma)\phi^*_{k's'}(\boldsymbol{r}'\sigma')\left\{c_{ks}, c^\dagger_{k's'}\right\} = \delta_{\sigma\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}') \quad (1.15)$$

Note that

$$\{\psi(\boldsymbol{r}\sigma), \psi(\boldsymbol{r}'\sigma')\} = 0 \quad (1.16)$$

2-body wave function

Using the expression of the Slater determinant in the second quantization, 2-body wave function is given by

$$\begin{aligned}\Phi_{k_1,k_2}(\boldsymbol{r}_1,\boldsymbol{r}_2) &= \frac{1}{\sqrt{2}}\langle \boldsymbol{r}_1,\boldsymbol{r}_2|c^\dagger_{k_1}c^\dagger_{k_2}|-\rangle \\ &= \frac{1}{\sqrt{2}}\langle \boldsymbol{r}_1,\boldsymbol{r}_2|1_{k_1},1_{k_2}\rangle_a \quad (1.17)\end{aligned}$$

In terms of the coordinate space field operator,$|\boldsymbol{r}_1,\boldsymbol{r}_2\rangle$ can be expressed as

$$|\boldsymbol{r}_1,\boldsymbol{r}_2\rangle = \psi^\dagger(\boldsymbol{r}_1)\psi^\dagger(\boldsymbol{r}_2)|-\rangle \quad (1.18)$$

Hence

$$\begin{aligned}\Phi_{k_1,k_2}(\boldsymbol{r}_1,\boldsymbol{r}_2) &= \frac{1}{\sqrt{2}}\langle \boldsymbol{r}_1,\boldsymbol{r}_2|c^\dagger_{k_1}c^\dagger_{k_2}|-\rangle \\ &= \frac{1}{\sqrt{2}}\langle -|\psi(\boldsymbol{r}_2)\psi(\boldsymbol{r}_1)c^\dagger_{k_2}c^\dagger_{k_2}|-\rangle \\ &= \frac{1}{\sqrt{2}}\left(\phi_{k_1}(\boldsymbol{r}_1)\phi_{k_2}(\boldsymbol{r}_2) - \phi_{k_2}(\boldsymbol{r}_1)\phi_{k_1}(\boldsymbol{r}_2)\right) = \frac{1}{\sqrt{2}}\begin{vmatrix} \phi_{k_1}(\boldsymbol{r}_1) & \phi_{k_1}(\boldsymbol{r}_2) \\ \phi_{k_2}(\boldsymbol{r}_1) & \phi_{k_2}(\boldsymbol{r}_2)\end{vmatrix} \quad (1.19)\end{aligned}$$

1.1.3 1-particle operator and 2-particle operator

In general, a Hamiltonian is given by

$$\begin{aligned}\hat{\mathrm{H}} &= \sum_i \frac{\hat{p}_i^2}{2m} + \sum_{i<j}\hat{v}(\boldsymbol{r}_i,\boldsymbol{r}_j) \quad (1.20)\\ &= \sum_i \frac{\hat{p}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j}\hat{v}(\boldsymbol{r}_i,\boldsymbol{r}_j) \quad (1.21)\end{aligned}$$

in the quantum mechanics.(Here we neglect spin.) In this Hamiltonian, the first term, the kinetic energy term, is the 1-particle operator. The second term, the interaction term, is the 2-particle operator.

Generally, as seen in the Hamiltonian, 1-particle and 2-particle operators take the form thus

$$\hat{F} \equiv \sum_i \hat{f}(\boldsymbol{r}_i) \qquad \text{(1-particle operator)} \quad (1.22)$$

$$\hat{V} \equiv \frac{1}{2}\sum_{i\neq j} v(\boldsymbol{r}_i,\boldsymbol{r}_j) = \sum_{i<j}\hat{v}(\boldsymbol{r}_i,\boldsymbol{r}_j) \qquad \text{(2-particle operator)} \quad (1.23)$$

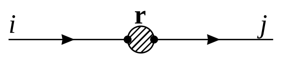
Using the coordinate space representation of the field operator, 1-body and 2-body operators in the coordinate space representation are given by

$$\hat{F} \equiv \sum_{ij} f_{ij}c^\dagger_i c_j = \int d\boldsymbol{r}\psi^\dagger(\boldsymbol{r})\hat{f}(\boldsymbol{r})\psi(\boldsymbol{r}) \quad (1.27)$$

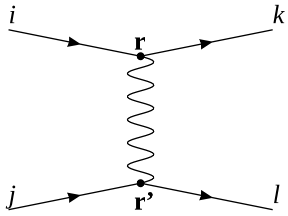
$$\hat{V} \equiv \frac{1}{2}\sum_{ijkl} v_{ijkl}c^\dagger_i c^\dagger_j c_l c_k = -\frac{1}{2}\int\int d\boldsymbol{r}d\boldsymbol{r}'\psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\hat{v}(\boldsymbol{r},\boldsymbol{r}')\psi(\boldsymbol{r})\psi(\boldsymbol{r}') \quad (1.28)$$

The matrix elements of these operators are defined as

$$
\begin{aligned}
\langle i|\hat{f}|j\rangle &\equiv \int d\boldsymbol{r}\phi_i^*(\boldsymbol{r})\hat{f}(\boldsymbol{r})\phi_j(\boldsymbol{r}) \\
&\equiv f_{ij} \qquad (1.24) \\
\langle ij|\hat{v}|kl\rangle &\equiv \int\int d\boldsymbol{r}d\boldsymbol{r}'\phi_i^*(\boldsymbol{r})\phi_j^*(\boldsymbol{r}')\hat{v}(\boldsymbol{r},\boldsymbol{r}')\phi_k(\boldsymbol{r})\phi_l(\boldsymbol{r}') \\
&\equiv v_{ijkl} \qquad (1.25)
\end{aligned}
$$



Second quantization rule for the 1,2-body operators



Using the matrix elements of operators, the second quantization rule for operators can be given **so as to obtain the same expectation value and matrix elements for $\hat{F}$ and $\hat{V}$**, thus

$$
\begin{aligned}
\hat{F} \equiv \sum_i \hat{f}(\boldsymbol{r}_i) \quad &\rightarrow \quad \hat{F} \equiv \sum_{ij} f_{ij} c_i^\dagger c_j \\
\hat{V} \equiv \frac{1}{2}\sum_{i\neq j} \hat{v}(\boldsymbol{r}_i,\boldsymbol{r}_j) \quad &\rightarrow \quad \hat{V} \equiv \frac{1}{2}\sum_{ijkl} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k
\end{aligned} \qquad (1.26)
$$

In many calculations the evaluation of the matrix elements leads to an antisymmetric combination, which is threfore given a special abbreviation:

$$\tilde{v}_{ijkl} \equiv v_{ijkl} - v_{ijlk} \qquad (1.29)$$

Using this abbreviation,

$$\sum_{ijkl} \tilde{v}_{ijkl} c_i^\dagger c_j^\dagger c_l c_k = \sum_{ijkl} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k - \sum_{ijkl} v_{ijlk} c_i^\dagger c_j^\dagger c_l c_k = 2\sum_{ijkl} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k \qquad (1.30)$$

Then 2-particle operator can be written as

$$
\begin{aligned}
\hat{V} &\equiv \frac{1}{2}\sum_{ijkl} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k = \frac{1}{4}\sum_{ijkl} \tilde{v}_{ijkl} c_i^\dagger c_j^\dagger c_l c_k \qquad (1.31) \\
&= -\frac{1}{2}\int\int d\boldsymbol{r}d\boldsymbol{r}'\psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\hat{v}(\boldsymbol{r},\boldsymbol{r}')\psi(\boldsymbol{r})\psi(\boldsymbol{r}') \qquad (1.32) \\
&= \frac{1}{4}\int\int d\boldsymbol{r}d\boldsymbol{r}'\psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\hat{v}(\boldsymbol{r},\boldsymbol{r}')\left(\psi(\boldsymbol{r}')\psi(\boldsymbol{r}) - \psi(\boldsymbol{r})\psi(\boldsymbol{r}')\right) \qquad (1.33) \\
&= \frac{1}{4}\int\int d\boldsymbol{r}d\boldsymbol{r}'\psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\hat{v}(\boldsymbol{r},\boldsymbol{r}')\left(1 - \mathrm{P}_r\right)\psi(\boldsymbol{r}')\psi(\boldsymbol{r}) \qquad (1.34) \\
&= \frac{1}{4}\int\int d\boldsymbol{r}d\boldsymbol{r}'\psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\tilde{v}(\boldsymbol{r},\boldsymbol{r}')\psi(\boldsymbol{r}')\psi(\boldsymbol{r}) \qquad (1.35)
\end{aligned}
$$

Then a Hamiltonian can be expressed in the second quantization representation:

$$
\begin{aligned}
\hat{\mathrm{H}} &= \sum_{ij}\langle i|\frac{-\hbar^2}{2m}\nabla^2|j\rangle c_i^\dagger c_j + \frac{1}{4}\sum_{i\neq j}\langle ij|\tilde{v}(\boldsymbol{r},\boldsymbol{r}')|kl\rangle c_i^\dagger c_j^\dagger c_l c_k \qquad (1.36) \\
&= \int d\boldsymbol{r}\psi^\dagger(\boldsymbol{r})\frac{-\hbar^2}{2m}\nabla^2\psi(\boldsymbol{r}) + \frac{1}{4}\int\int d\boldsymbol{r}d\boldsymbol{r}'\psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\tilde{v}(\boldsymbol{r},\boldsymbol{r}')\psi(\boldsymbol{r}')\psi(\boldsymbol{r}) \qquad (1.37)
\end{aligned}
$$

Isovector type and Isoscalar type 1-body operator

In general, the isoscalar type and isovector type operator take the form as

$$
\begin{aligned}
&\text{Isoscalar type:}(T=0) \qquad \sum_i f(\boldsymbol{r}_i) \\
&\text{Isoscalar type:}(T=1) \qquad \sum_i \tau_z(i) f(\boldsymbol{r}_i)
\end{aligned}
$$

where τ_z is the 3rd component isospin operator,

$$\frac{1}{2}\tau_z = t_z \qquad t_z|p\rangle = -\frac{1}{2}|p\rangle \qquad t_z|n\rangle = \frac{1}{2}|n\rangle$$

Then the 2nd quantized expressions are

$$\begin{aligned}\hat{F}_{IS} &= \sum_{tau=-1,1} \int d\boldsymbol{r}\psi^\dagger(\boldsymbol{r}\tau)f(\boldsymbol{r})\psi(\boldsymbol{r}\tau) = \int d\boldsymbol{r}\psi_n^\dagger(\boldsymbol{r})f(\boldsymbol{r})\psi_n(\boldsymbol{r}) + \int d\boldsymbol{r}\psi_p^\dagger(\boldsymbol{r})f(\boldsymbol{r})\psi_p(\boldsymbol{r}) \\ \hat{F}_{IV} &= \sum_{tau=-1,1} \int d\boldsymbol{r}\psi^\dagger(\boldsymbol{r}\tau)\tau_z f(\boldsymbol{r})\psi(\boldsymbol{r}\tau) = \int d\boldsymbol{r}\psi_n^\dagger(\boldsymbol{r})f(\boldsymbol{r})\psi_n(\boldsymbol{r}) - \int d\boldsymbol{r}\psi_p^\dagger(\boldsymbol{r})f(\boldsymbol{r})\psi_p(\boldsymbol{r})\end{aligned}$$

1.2 Density matrics

The density $\rho(\boldsymbol{r})$ can be expressed by using the single-particle wave function as

$$\rho(\boldsymbol{r}) = \sum_{i\ni hole,\sigma} |\phi_i(\boldsymbol{r}\sigma)|^2 \tag{1.38}$$

$$= \sum_{k\leq k_F,\sigma} |\phi_k(\boldsymbol{r}\sigma)|^2 \tag{1.39}$$

$$= \sum_{i=1}^{N}\sum_{\sigma} |\phi_i(\boldsymbol{r}\sigma)|^2 \tag{1.40}$$

1.2.1 The density operator

Quantum mechanics representation

The density can be also expressed by using the Slater determinant.

$$\rho(\boldsymbol{r}) = \sum_{i=1}^{N} |\phi_{k_i}(\boldsymbol{r})|^2 \tag{1.41}$$

$$= \int\cdots\int d\boldsymbol{r}_1\ldots d\boldsymbol{r}_N \Phi^*_{\{k_1\ldots k_N\}}(\boldsymbol{r}_1\ldots\boldsymbol{r}_N)\left[\delta(\boldsymbol{r}-\boldsymbol{r}_1)+\ldots+\delta(\boldsymbol{r}-\boldsymbol{r}_N)\right]\Phi_{\{k_1\ldots k_N\}}(\boldsymbol{r}_1\ldots\boldsymbol{r}_N)$$

$$= \int\cdots\int d\boldsymbol{r}_1\ldots d\boldsymbol{r}_N \Phi^*_{\{k_1\ldots k_N\}}(\boldsymbol{r}_1\ldots\boldsymbol{r}_N)\left[\sum_{i=1}^{N}\delta(\boldsymbol{r}-\boldsymbol{r}_i)\right]\Phi_{\{k_1\ldots k_N\}}(\boldsymbol{r}_1\ldots\boldsymbol{r}_N) \tag{1.42}$$

$$= \langle\Phi|\left[\sum_{i=1}^{N}\delta(\boldsymbol{r}-\boldsymbol{r}_i)\right]|\Phi\rangle \tag{1.43}$$

Hence we can define the density operator like as

$$\hat{\rho}(\boldsymbol{r}) \equiv \sum_{i=1}^{N}\delta(\boldsymbol{r}-\boldsymbol{r}_i) \tag{1.44}$$

in the quantum mechanics.

Second Quantization representation

Under the second quantization rule, the density operator can be defined

$$\hat{\rho}(\boldsymbol{r}) \equiv \sum_{ij} d_{ij}c_i^\dagger c_j = \psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}) \tag{1.45}$$

$$\text{where} \quad \begin{aligned} d_{ij} &= \langle i|\delta(\boldsymbol{r}-\hat{\boldsymbol{r}})|j\rangle \\ &= \int d\boldsymbol{r}'\phi_i^*(\boldsymbol{r}')\delta(\boldsymbol{r}-\hat{\boldsymbol{r}})\phi_j(\boldsymbol{r}') = \phi_i^*(\boldsymbol{r})\phi_j(\boldsymbol{r})\end{aligned} \tag{1.46}$$

Note that $\hat{\boldsymbol{r}}$ is a coordinate operator, *i.e.*

$$\begin{aligned}\hat{\boldsymbol{r}}\phi_j(\boldsymbol{r}') &= \langle\boldsymbol{r}'|\hat{\boldsymbol{r}}|j\rangle = \boldsymbol{r}'\langle\boldsymbol{r}'|j\rangle \\ &= \boldsymbol{r}'\phi_j(\boldsymbol{r}')\end{aligned}$$

Using this density operator, its expectation value is the normal density.

$$\begin{aligned} \langle 0|\hat{\rho}(\boldsymbol{r})|0\rangle &= \langle 0|\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r})|0\rangle = \sum_{ij}\phi_i^*(\boldsymbol{r})\phi_j(\boldsymbol{r})\langle 0|c_i^\dagger c_j|0\rangle & (1.47)\\ &= \sum_{ij}\phi_j(\boldsymbol{r})\rho_{ji}\phi_i^*(\boldsymbol{r}) = \sum_{i\in hole}|\phi_i(\boldsymbol{r})|^2 = \rho(\boldsymbol{r}) & (1.48)\\ &\text{where}\quad \rho_{ji}\equiv\langle 0|c_i^\dagger c_j|0\rangle \quad (=\theta(k_F-k_i)\delta_{ij}) & (1.49)\end{aligned}$$

Here we defined the density matrix ρ_{ji} in the configuration space representation. (But in the ground state, the density matrix in the configuration space has only the diagonal element for hole states.) In the coordinate space representation, we can also define the density matrix.

$$\begin{aligned} \rho(\boldsymbol{r},\boldsymbol{r}') &\equiv \langle 0|\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r})|0\rangle & (1.50)\\ &= \sum_{ij}\phi_j(\boldsymbol{r})\rho_{ji}\phi_i^*(\boldsymbol{r}') = \sum_{i\in hole}\phi_i(\boldsymbol{r})\phi_i^*(\boldsymbol{r}') & (1.51)\end{aligned}$$

1.2.2 Density matrix with spin indices and Spin density

Here we define the density matrix for the spin component and also can define the spin density ρ_i.

$$\rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma')\equiv\boldsymbol{\rho}(\boldsymbol{r}\boldsymbol{r}')_{\sigma\sigma'}=\frac{1}{2}\left(\rho(\boldsymbol{r}\boldsymbol{r}')\delta_{\sigma\sigma'}+\sum_i\langle\sigma|\sigma_i|\sigma'\rangle\rho_i(\boldsymbol{r}\boldsymbol{r}')\right) \quad (1.52)$$

i.e.

$$\boldsymbol{\rho}(\boldsymbol{r}\boldsymbol{r}')=\frac{1}{2}\begin{pmatrix}\rho(\boldsymbol{r}\boldsymbol{r}')+\rho_z(\boldsymbol{r}\boldsymbol{r}') & \rho_x(\boldsymbol{r}\boldsymbol{r}')-i\rho_y(\boldsymbol{r}\boldsymbol{r}')\\ \rho_x(\boldsymbol{r}\boldsymbol{r}')+i\rho_y(\boldsymbol{r}\boldsymbol{r}') & \rho(\boldsymbol{r}\boldsymbol{r}')-\rho_z(\boldsymbol{r}\boldsymbol{r}')\end{pmatrix}=\frac{1}{2}\left(\mathbf{1}\rho(\boldsymbol{r}\boldsymbol{r}')+\boldsymbol{\sigma}\cdot\boldsymbol{\rho}(\boldsymbol{r}\boldsymbol{r}')\right) \quad (1.53)$$

where

$$\mathbf{1}=\begin{pmatrix}1&0\\0&1\end{pmatrix}\qquad\sigma_x=\begin{pmatrix}0&1\\1&0\end{pmatrix}\qquad\sigma_y=\begin{pmatrix}0&-i\\i&0\end{pmatrix}\qquad\sigma_z=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

$$\mathbf{1}_{\sigma\sigma'}=\delta_{\sigma\sigma'}\qquad(\sigma_x)_{\sigma\sigma'}=\langle\sigma|\sigma_x|\sigma'\rangle\qquad(\sigma_y)_{\sigma\sigma'}=\langle\sigma|\sigma_y|\sigma'\rangle\qquad(\sigma_z)_{\sigma\sigma'}=\langle\sigma|\sigma_z|\sigma'\rangle$$

Using the Pauli-matrices properties the inverce relations are obtained as

$$\begin{aligned} \rho(\boldsymbol{r}\boldsymbol{r}') &= \sum_{\sigma\sigma'}\delta_{\sigma\sigma'}\rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma')=\sum_{\sigma}\rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma)=\mathrm{Tr}[\boldsymbol{\rho}(\boldsymbol{r},\boldsymbol{r}')]\left(\equiv\frac{1}{2}\rho_{00}(\boldsymbol{r}\boldsymbol{r}')\right) & (1.54)\\ \rho_i(\boldsymbol{r}\boldsymbol{r}') &= \sum_{\sigma\sigma'}\langle\sigma'|\sigma_i|\sigma\rangle\rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma')=\left\{\begin{array}{l}\rho_x(\boldsymbol{r}\boldsymbol{r}')=(\rho(\boldsymbol{r}\uparrow,\boldsymbol{r}'\downarrow)+\rho(\boldsymbol{r}\downarrow,\boldsymbol{r}'\uparrow))\\ \rho_y(\boldsymbol{r}\boldsymbol{r}')=i\,(\rho(\boldsymbol{r}\uparrow,\boldsymbol{r}'\downarrow)-\rho(\boldsymbol{r}\downarrow,\boldsymbol{r}'\uparrow))\\ \rho_z(\boldsymbol{r}\boldsymbol{r}')=(\rho(\boldsymbol{r}\uparrow,\boldsymbol{r}'\uparrow)-\rho(\boldsymbol{r}\downarrow,\boldsymbol{r}'\downarrow))\end{array}\right. & (1.55)\\ &= \mathrm{Tr}\left[\sigma_i\boldsymbol{\rho}(\boldsymbol{r}\boldsymbol{r}')\right](\equiv 2\rho_{10,i}(\boldsymbol{r}\boldsymbol{r}')) & (1.56)\end{aligned}$$

In addition, if one considers the isospin indices, then

$$\begin{aligned} \rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma'\tau') &= \frac{1}{2}\rho(\boldsymbol{r}\tau,\boldsymbol{r}'\tau')\delta_{\sigma\sigma'}+\frac{1}{2}\sum_i\langle\sigma|\sigma_i|\sigma'\rangle\rho_i(\boldsymbol{r}\tau,\boldsymbol{r}'\tau') & (1.57)\\ &= \frac{1}{2}\left(\frac{1}{2}\rho(\boldsymbol{r},\boldsymbol{r}')\delta_{\tau\tau'}+\frac{1}{2}\sum_j\langle\tau|\tau_j|\tau'\rangle\rho_{0,j}(\boldsymbol{r},\boldsymbol{r}')\right)\delta_{\sigma\sigma'} & (1.58)\\ &\quad+\frac{1}{2}\sum_i\langle\sigma|\sigma_i|\sigma'\rangle\left(\frac{1}{2}\rho_{i,0}(\boldsymbol{r},\boldsymbol{r}')\delta_{\tau\tau'}+\frac{1}{2}\sum_j\langle\tau|\tau_j|\tau'\rangle\rho_{i,j}(\boldsymbol{r},\boldsymbol{r}')\right) & (1.59)\\ &= \frac{1}{4}\rho(\boldsymbol{r},\boldsymbol{r}')\delta_{\tau\tau'}\delta_{\sigma\sigma'}+\frac{1}{4}\sum_j\langle\tau|\tau_j|\tau'\rangle\rho_{0,j}(\boldsymbol{r},\boldsymbol{r}')\delta_{\sigma\sigma'} & (1.60)\\ &\quad+\frac{1}{4}\sum_i\langle\sigma|\sigma_i|\sigma'\rangle\rho_{i,0}(\boldsymbol{r},\boldsymbol{r}')\delta_{\tau\tau'}+\frac{1}{4}\sum_{i,j}\langle\sigma|\sigma_i|\sigma'\rangle\langle\tau|\tau_j|\tau'\rangle\rho_{i,j}(\boldsymbol{r},\boldsymbol{r}') & (1.61)\end{aligned}$$

where

$$\begin{aligned}
\mathrm{Tr}[\tau_k\rho] &= \sum_{\tau,\tau'}\langle\tau'|\tau_k|\tau\rangle\rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma'\tau') \\
&= \frac{1}{2}\rho_{0,k}(\boldsymbol{r}\boldsymbol{r}')\delta_{\sigma\sigma'}+\frac{1}{2}\sum_i\langle\sigma|\sigma_i|\sigma'\rangle\rho_{i,k}(\boldsymbol{r}\boldsymbol{r}') \\
\mathrm{Tr}[\sigma_k\rho] &= \sum_{\sigma,\sigma'}\langle\sigma'|\sigma_k|\sigma\rangle\rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma'\tau') \\
&= \frac{1}{2}\rho_{k,0}(\boldsymbol{r}\boldsymbol{r}')\delta_{\tau\tau'}+\frac{1}{2}\sum_i\langle\tau|\tau_i|\tau'\rangle\rho_{k,i}(\boldsymbol{r}\boldsymbol{r}') \\
\mathrm{Tr}[\sigma_k\tau_l\rho] &= \sum_{\sigma,\sigma'}\sum_{\tau,\tau'}\langle\sigma'|\sigma_k|\sigma\rangle\langle\tau'|\tau_l|\tau\rangle\rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma'\tau') = \rho_{k,l}(\boldsymbol{r}\boldsymbol{r}')
\end{aligned}$$

1.3 Time reversal symmetry

Time reversal symmetry is supposed in the ground state of nuclei, then the density matrix has the property:

$$\begin{aligned}
\rho^*(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') &= \langle\Phi|\psi^\dagger(\boldsymbol{r}'\sigma')\psi(\boldsymbol{r}\sigma)|\Phi\rangle^* && (1.62)\\
&= \langle\Phi|\mathcal{T}\mathcal{T}^\dagger\psi^\dagger(\boldsymbol{r}'\sigma')\mathcal{T}\mathcal{T}^\dagger\psi(\boldsymbol{r}\sigma)\mathcal{T}\mathcal{T}^\dagger|\Phi\rangle && (1.63)\\
&= \langle\mathcal{T}^\dagger\Phi|\left(-2\sigma'\psi^\dagger(\boldsymbol{r}'-\sigma')\right)\left(-2\sigma\psi(\boldsymbol{r}-\sigma)\right)|\mathcal{T}\Phi\rangle && (1.64)\\
&= 4\sigma\sigma'\rho(\boldsymbol{r}-\sigma,\boldsymbol{r}'-\sigma') && (1.65)
\end{aligned}$$

On the other hand, the density matrix is the hermite matrix.

$$\rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma')^* = \rho(\boldsymbol{r}'\sigma',\boldsymbol{r}\sigma) \quad (1.66)$$

Thus

$$\rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') = \frac{1}{2}\left(\rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma')+4\sigma\sigma'\rho(\boldsymbol{r}'-\sigma',\boldsymbol{r}-\sigma)\right) \quad (1.67)$$

$$\to \frac{1}{4}\left\{\begin{pmatrix}\rho(\boldsymbol{r}\boldsymbol{r}')+\rho_z(\boldsymbol{r}\boldsymbol{r}') & \rho_x(\boldsymbol{r}\boldsymbol{r}')-i\rho_y(\boldsymbol{r}\boldsymbol{r}')\\ \rho_x(\boldsymbol{r}\boldsymbol{r}')+i\rho_y(\boldsymbol{r}\boldsymbol{r}') & \rho(\boldsymbol{r}\boldsymbol{r}')-\rho_z(\boldsymbol{r}\boldsymbol{r}')\end{pmatrix}\right. \quad (1.68)$$

$$\left.+\begin{pmatrix}\rho(\boldsymbol{r}'\boldsymbol{r})-\rho_z(\boldsymbol{r}'\boldsymbol{r}) & -\rho_x(\boldsymbol{r}'\boldsymbol{r})+i\rho_y(\boldsymbol{r}'\boldsymbol{r})\\ -\rho_x(\boldsymbol{r}'\boldsymbol{r})-i\rho_y(\boldsymbol{r}'\boldsymbol{r}) & \rho(\boldsymbol{r}'\boldsymbol{r})+\rho_z(\boldsymbol{r}'\boldsymbol{r})\end{pmatrix}\right\} = \frac{1}{2}\begin{pmatrix}\rho(\boldsymbol{r}\boldsymbol{r}') & 0\\ 0 & \rho(\boldsymbol{r}\boldsymbol{r}')\end{pmatrix} \quad (1.69)$$

where we suppose $\rho(\boldsymbol{r}\boldsymbol{r}')=\rho(\boldsymbol{r}'\boldsymbol{r}) \quad \rho_i(\boldsymbol{r}\boldsymbol{r}')=\rho_i(\boldsymbol{r}'\boldsymbol{r})$

Consequently, under the time reversal symmetry the spin density is vanished.

$$\rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') = \frac{1}{2}\rho(\boldsymbol{r}\boldsymbol{r}')\delta_{\sigma\sigma'} \quad (1.70)$$

1.4 Wick's theorem

Construction and Normal order

The construction symbol $\overbrace{AB}$, which is used in wick's theorem, is defined as

$$\overbrace{\psi^\dagger(x)\psi}(y) \equiv \langle\Phi|\psi^\dagger(x)\psi(y)|\Phi\rangle \quad (1.71)$$

The *normal order* ": AB :" is defined so as to be

$$\langle\Phi| : AB : |\Phi\rangle = 0 \quad (1.72)$$

for some kinds of vacuum $|\Phi\rangle$.

Example of the normal order

In the Hartree-Fock approximation, the mean field Hamiltonian can be expressed by using normal order like as

$$\hat{h}_0 = \sum_k \epsilon_k : c_k^\dagger c_k : \left(= \sum_k \epsilon_k c_k^\dagger c_k \quad \text{for the vacuum } |-\rangle \right) \tag{1.73}$$

$$= \sum_{k>k_F} \epsilon_k : a_k^\dagger a_k : + \sum_{k\leq k_F} \epsilon_k : b_k b_k^\dagger :$$

$$= \sum_{k>k_F} \epsilon_k a_k^\dagger a_k - \sum_{k\leq k_F} \epsilon_k b_k^\dagger b_k \quad \text{for the fermi vacuum } |0\rangle \tag{1.74}$$

Wick's theorem for 2 or 4 operators can be given by

$$AB =: AB : + \overline{AB} \qquad ABCD = \; : ABCD : + : \overline{AB}CD : + : \overline{ABC}D : + : \overline{ABCD} :$$

$$+ : A\overline{BC}D : + : A\overline{BCD} : + : AB\overline{CD} :$$

$$+ : \overline{AB}\,\overline{CD} : + : \overline{ABC}\!\!\!\!\!\!\overline{CD} : + : \overline{A\overline{BC}D} :$$

$$= \; : ABCD : + \overline{AB} : CD : - \overline{AC} : BD : + \overline{AD} : BC :$$

$$+ \overline{BC} : AD : - \overline{BD} : AC : + \overline{CD} : AB :$$

$$+ \overline{AB}\,\overline{CD} - \overline{AC}\,\overline{BD} + \overline{AD}\,\overline{BC} \tag{1.75}$$

Note that the expansion by Wick's theorem for the operators in the Hamiltonian is

$$c_k^\dagger c_{k'} \begin{cases} = \; : c_k^\dagger c_{k'} : \; = c_k^\dagger c_{k'} & \text{(for the vacuum } |-\rangle) \\ = \; : c_k^\dagger c_{k'} : + \overline{c_k^\dagger c_{k'}} & \text{(for the fermi vacuum } |0\rangle) \end{cases}$$

$$= \theta(k - k_F) : a_k^\dagger a_{k'} : - \theta(k_F - k) : b_k^\dagger b_{k'} : + \theta(k_F - k)\delta_{kk'}$$

$$c_{k_1}^\dagger c_{k_2}^\dagger c_{k_4} c_{k_3} \begin{cases} = \; : c_{k_1}^\dagger c_{k_2}^\dagger c_{k_4} c_{k_3} : \; = c_{k_1}^\dagger c_{k_2}^\dagger c_{k_4} c_{k_3} & \text{(for the vacuum } |-\rangle) \\ = \; : c_{k_1}^\dagger c_{k_2}^\dagger c_{k_4} c_{k_3} : & \\ \quad + \overline{c_{k_1}^\dagger c_{k_3}} : c_{k_2}^\dagger c_{k_4} : - \overline{c_{k_1}^\dagger c_{k_4}} : c_{k_2}^\dagger c_{k_3} : + \overline{c_{k_2}^\dagger c_{k_4}} : c_{k_1}^\dagger c_{k_3} : - \overline{c_{k_2}^\dagger c_{k_3}} : c_{k_1}^\dagger c_{k_4} : & \\ \quad + \overline{c_{k_1}^\dagger c_{k_3}}\,\overline{c_{k_2}^\dagger c_{k_4}} - \overline{c_{k_1}^\dagger c_{k_4}}\,\overline{c_{k_2}^\dagger c_{k_3}} & \text{(for the fermi vacuum } |0\rangle) \end{cases}$$

Interpretation of the construction of the density operator

The Wick's construction of the density operator $\psi^\dagger(x)\psi(x)$ gives **the expectation value of the density operator for some vacuum.**

$$\overline{\psi^\dagger(x)\psi(x)} = \begin{cases} \langle -|\psi^\dagger(x)\psi(x)|-\rangle = 0 & : |-\rangle \text{ is the exact vacuum.(no particle)} \\ \langle \Phi|\psi^\dagger(x)\psi(x)|\Phi\rangle = \rho(x) & : |\Phi\rangle \text{ is the (Hartree-Fock) Fermi vacuum. (no particle and no hole)} \end{cases}$$

1.5 Hartree-Fock arroximation

Using Wick's theorem expansion, the Hamiltonian can be expanded for the Fermi vacuum,

$$\hat{\mathrm{H}} = \sum_{ij} \langle i|\frac{-\hbar^2}{2m}\nabla^2|j\rangle c_i^\dagger c_j + \frac{1}{4}\sum_{i\neq j}\sum_{k\neq l} \langle ij|\tilde{v}(\boldsymbol{r},\boldsymbol{r}')|kl\rangle c_i^\dagger c_j^\dagger c_l c_k \tag{1.76}$$

$$= \sum_{k_i\leq k_F} \langle i|\frac{-\hbar^2}{2m}\nabla^2|i\rangle + \frac{1}{4}\sum_{(k_i,k_j)\leq k_F} \left(\langle ij|\tilde{v}(\boldsymbol{r},\boldsymbol{r}')|ij\rangle - \langle ij|\tilde{v}(\boldsymbol{r},\boldsymbol{r}')|ji\rangle\right)$$

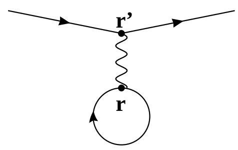
$$+ \sum_{i,j} \langle i|\frac{-\hbar^2}{2m}\nabla^2|j\rangle : c_i^\dagger c_j :$$

$$+ \frac{1}{4}\sum_{k\leq k_F}\sum_{i,j} \left(\langle ki|\tilde{v}(\boldsymbol{r},\boldsymbol{r}')|kj\rangle - \langle ki|\tilde{v}(\boldsymbol{r},\boldsymbol{r}')|jk\rangle\right) : c_i^\dagger c_j :$$

$$
\begin{aligned}
&+\frac{1}{4}\sum_{k\le k_F}\sum_{i,j}\left(\langle ik|\tilde{v}(\boldsymbol{r},\boldsymbol{r}')|jk\rangle - \langle ik|\tilde{v}(\boldsymbol{r},\boldsymbol{r}')|kj\rangle\right) : c_i^\dagger c_j : \\
&+(\textit{residual int. term}) \qquad (1.77)\\
= &\sum_{k_i\le k_F}\frac{\hbar^2}{2m}\int d\boldsymbol{r}|\nabla\phi_i(\boldsymbol{r})|^2 + \frac{1}{2}\sum_{(k_i,k_j)\le k_F}\iint d\boldsymbol{r}d\boldsymbol{r}'\phi_i^*(\boldsymbol{r})\phi_j^*(\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')\left(\phi_i(\boldsymbol{r})\phi_j(\boldsymbol{r}') - \phi_j(\boldsymbol{r})\phi_i(\boldsymbol{r}')\right)\\
&+\int d\boldsymbol{r} : \psi^\dagger(\boldsymbol{r})\frac{-\hbar^2}{2m}\nabla^2\psi^\dagger(\boldsymbol{r}) :\\
&+ : \int d\boldsymbol{r}'\psi^\dagger(\boldsymbol{r}')\left[\int d\boldsymbol{r}\sum_{k\le k_F}\phi_k^*(\boldsymbol{r})v(\boldsymbol{r},\boldsymbol{r}')\phi_k(\boldsymbol{r})\right]\psi(\boldsymbol{r}') : - \iint d\boldsymbol{r}d\boldsymbol{r}' : \psi^\dagger(\boldsymbol{r}')\sum_{k\le k_F}\phi_k^*(\boldsymbol{r})v(\boldsymbol{r},\boldsymbol{r}')\phi_k(\boldsymbol{r}')\psi(\boldsymbol{r}) :\\
&+(\textit{residual int. term}) \qquad (1.78)
\end{aligned}
$$

If we suppose that $v(\boldsymbol{r},\boldsymbol{r}')$ includes no exchange operaters, the Hamiltonian can be rewritten again as:

$$
\begin{aligned}
\hat{H} \;\rightarrow\; &\left[\int d\boldsymbol{r}\frac{\hbar^2}{2m}\tau(\boldsymbol{r}) + \frac{1}{2}\iint d\boldsymbol{r}d\boldsymbol{r}'\rho(\boldsymbol{r})v(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}') - \frac{1}{2}\iint d\boldsymbol{r}d\boldsymbol{r}'\rho^*(\boldsymbol{r}'\boldsymbol{r})v(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}'\boldsymbol{r})\right]\\
&+\int d\boldsymbol{r} : \psi^\dagger(\boldsymbol{r})\frac{-\hbar^2}{2m}\nabla^2\psi^\dagger(\boldsymbol{r}) :\\
&+ : \int d\boldsymbol{r}'\psi^\dagger(\boldsymbol{r}')\left[\int d\boldsymbol{r}\rho(\boldsymbol{r})v(\boldsymbol{r},\boldsymbol{r}')\right]\psi(\boldsymbol{r}') : - \iint d\boldsymbol{r}d\boldsymbol{r}' : \psi^\dagger(\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}'\boldsymbol{r})\psi(\boldsymbol{r}) :\\
&+(\textit{residual int. term})
\end{aligned}
$$



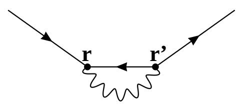
Direct term

where

$$
: \int d\boldsymbol{r}'\psi^\dagger(\boldsymbol{r}')\left[\int d\boldsymbol{r}\rho(\boldsymbol{r})v(\boldsymbol{r},\boldsymbol{r}')\right]\psi(\boldsymbol{r}') : \qquad \text{Direct term}
$$

$$
-\iint d\boldsymbol{r}d\boldsymbol{r}' : \psi^\dagger(\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}'\boldsymbol{r})\psi(\boldsymbol{r}) : \qquad \text{Exchange term}
$$

These terms can be represented by *Feynman diagram* as seen in the left figures.(The upper figure is the "direct term", the lower figure is the "exchange term")



Exchange term

1.5.1 Mean field Hamiltonian and Hartree-Fock equation

Here we define the Hartree-Fock mean field $h(\boldsymbol{r}\boldsymbol{r}')$

$$
h(\boldsymbol{r}\boldsymbol{r}') \equiv \frac{\delta\langle H\rangle}{\delta\rho(\boldsymbol{r}'\boldsymbol{r})} \quad \text{where } \langle H\rangle = \left[\int d\boldsymbol{r}\frac{\hbar^2}{2m}\tau(\boldsymbol{r}) + \frac{1}{2}\iint d\boldsymbol{r}d\boldsymbol{r}'\rho(\boldsymbol{r})v(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}') - \frac{1}{2}\iint d\boldsymbol{r}d\boldsymbol{r}'\rho^*(\boldsymbol{r}'\boldsymbol{r})v(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}'\boldsymbol{r})\right]
$$

Hence

$$
\begin{aligned}
h(\boldsymbol{r}\boldsymbol{r}') &\equiv \frac{\delta\langle H\rangle}{\delta\rho(\boldsymbol{r}\boldsymbol{r}')}\\
&= \frac{\hbar^2}{2m}\int d\boldsymbol{r}''\nabla''\delta(\boldsymbol{r}''-\boldsymbol{r})\cdot\nabla''\delta(\boldsymbol{r}''-\boldsymbol{r}') + \int d\boldsymbol{r}''\rho(\boldsymbol{r}'')v(\boldsymbol{r}''\boldsymbol{r})\delta(\boldsymbol{r}-\boldsymbol{r}') - v(\boldsymbol{r}\boldsymbol{r}')\rho(\boldsymbol{r}'\boldsymbol{r})
\end{aligned}
$$

Then the Hamiltonian can be expressed by using the mean field

$$
\hat{H} = \langle H\rangle + \iint d\boldsymbol{r}d\boldsymbol{r}'h(\boldsymbol{r}\boldsymbol{r}') : \psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}') : +(\textit{residual int.}) \qquad (1.79)
$$

$$= \langle H \rangle + \iint d\boldsymbol{r} d\boldsymbol{r}' \sum_{k,k'} \phi_k^*(\boldsymbol{r}) h(\boldsymbol{r}\boldsymbol{r}') \phi_{k'}(\boldsymbol{r}') : c_k^\dagger c_{k'} : + (residual\ int.) \tag{1.80}$$

$$= \langle H \rangle + \iint d\boldsymbol{r} d\boldsymbol{r}' \sum_{k,k'} h_{kk'} : c_k^\dagger c_{k'} : + (residual\ int.) \tag{1.81}$$

The Hartree-Fock equation for the single-particle wave function is given by

$$\int d\boldsymbol{r}' h(\boldsymbol{r}\boldsymbol{r}') \phi_k(\boldsymbol{r}')$$
$$= \frac{-\hbar^2}{2m} \nabla^2 \phi_k(\boldsymbol{r}) + \left[\int d\boldsymbol{r}' \rho(\boldsymbol{r}') v(\boldsymbol{r}'\boldsymbol{r}) \right] \phi_k(\boldsymbol{r}) - \int d\boldsymbol{r}' v(\boldsymbol{r}\boldsymbol{r}') \rho(\boldsymbol{r}'\boldsymbol{r}) \phi_k(\boldsymbol{r}') = \epsilon_k \phi_k(\boldsymbol{r}) \tag{1.82}$$

which is based on the variational principle.

Consequently the Hamiltonian can be expressed as

$$\begin{aligned} \hat{H} &= \langle H \rangle + \sum_{k \in all} \epsilon_k : c_k^\dagger c_k : + (residual\ int.) \\ &= \langle H \rangle + \sum_{k > k_F} \epsilon_k a_k^\dagger a_k - \sum_{k \le k_F} \epsilon_k b_k^\dagger b_k + (residual\ int.) \\ &\rightarrow \langle H \rangle + \hat{h}_0 + (residual\ int.) \qquad \hat{h}_0 = \sum_{kk'} h_{kk'} : c_k^\dagger c_k := \sum_{kk'} \delta_{kk'} \epsilon_k : c_k^\dagger c_k : \end{aligned} \tag{1.83}$$

Note that

$$\hat{h}_0 |k\rangle = \begin{cases} \hat{h}_0 a_k^\dagger |0\rangle & = \sum_{k' > k_F} \epsilon_{k'} a_{k'}^\dagger a_{k'} a_k^\dagger |0\rangle & = \epsilon_k |k\rangle & (|k\rangle \text{ is a particle state. } i.e.\ k > k_F.) \\ \hat{h}_0 b_k^\dagger |0\rangle & = -\sum_{k' \le k_F} \epsilon_{k'} b_{k'}^\dagger b_{k'} b_k^\dagger |0\rangle & = -\epsilon_k |k\rangle & (|k\rangle \text{ is a hole state. } i.e.\ k \le k_F.) \end{cases}$$

This relation can be represented in the coordinate space.

$$\begin{aligned} \langle \boldsymbol{r} | \hat{h}_0 | k \rangle &= \langle - | \psi(\boldsymbol{r}) \iint d\boldsymbol{r}_1 d\boldsymbol{r}_2 h(\boldsymbol{r}_1 \boldsymbol{r}_2) \psi^\dagger(\boldsymbol{r}_1) \psi(\boldsymbol{r}_2) | k \rangle \\ &= \int d\boldsymbol{r}_2 h(\boldsymbol{r}\boldsymbol{r}_2) \langle - | \psi^\dagger(\boldsymbol{r}_2) | k \rangle \\ &= \int d\boldsymbol{r}_2 h(\boldsymbol{r}\boldsymbol{r}_2) \langle \boldsymbol{r}_2 | k \rangle = \pm \epsilon_k \langle \boldsymbol{r} | k \rangle \end{aligned}$$

This is the Hartree-Fock equation itself.

The mean field of the Coulomb interaction

In terms of the quantum mechanics, the Coulomb interction is given by

$$H_c = \frac{e^2}{4} \sum_{i<j} \frac{(1+\tau_{i3})(1+\tau_{j3})}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} \qquad \text{where} \qquad \tau_{i3} \phi(i,\tau) = \begin{cases} \phi_p(i) & (\tau = +1) \\ -\phi_n(i) & (\tau = -1) \end{cases} \tag{1.84}$$

Hence 2nd quantized Coulomb interaction is given by

$$\begin{aligned} H_c &= \frac{e^2}{8} \sum_{ijkl} \left[\sum_{\tau\tau'} \iint d\boldsymbol{r} d\boldsymbol{r}' \phi_i^*(\boldsymbol{r}\tau) \phi_j^*(\boldsymbol{r}'\tau') \frac{(1+\tau_3)(1+\tau_3')}{|\boldsymbol{r} - \boldsymbol{r}'|} \phi_k(\boldsymbol{r}\tau) \phi_l(\boldsymbol{r}'\tau') \right] c_i^\dagger c_j^\dagger c_l c_k \\ &= -\frac{e^2}{2} \iint d\boldsymbol{r} d\boldsymbol{r}' \psi_p^\dagger(\boldsymbol{r}) \psi_p^\dagger(\boldsymbol{r}') \frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|} \psi_p(\boldsymbol{r}) \psi_p(\boldsymbol{r}') \end{aligned} \tag{1.85}$$

Then

$$\langle H_c \rangle = -\frac{e^2}{2} \iint d\boldsymbol{r} d\boldsymbol{r}' \frac{[\rho_p(\boldsymbol{r}'\boldsymbol{r}) \rho_p(\boldsymbol{r}\boldsymbol{r}') - \rho_p(\boldsymbol{r}) \rho_p(\boldsymbol{r}')]}{|\boldsymbol{r} - \boldsymbol{r}'|} \tag{1.86}$$

$$\frac{\delta \langle H_c \rangle}{\delta \rho_p(\boldsymbol{r}'\boldsymbol{r})} = -e^2 \frac{\rho_p(\boldsymbol{r}\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} + e^2 \left[\frac{\int d\boldsymbol{r}_1 \rho_p(\boldsymbol{r}_1)}{|\boldsymbol{r} - \boldsymbol{r}_1|} \right] \delta(\boldsymbol{r} - \boldsymbol{r}') \tag{1.87}$$

The first term is so-called the "exchange term", which is often neglected in the H.F. calculation. The second term is the "direct term" of the Coulomb interaction.

1.6 Linear responce theory

The time dependent Schrödinger equation is

$$i\hbar\frac{\partial}{\partial t}|\Phi(t)\rangle = \hat{H}|\Phi(t)\rangle \tag{1.88}$$

Applying this equation to the (time-dependent) density we can get

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\rho(\boldsymbol{r};t) &= \langle\Phi(t)|\left[\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}), H\right]|\Phi(t)\rangle & (1.89)\\ &= \int d\boldsymbol{r}' \left(h(\boldsymbol{r}\boldsymbol{r}')\rho(\boldsymbol{r}',\boldsymbol{r};t) - \rho(\boldsymbol{r},\boldsymbol{r}';t)h(\boldsymbol{r}'\boldsymbol{r})\right) \qquad (= [h(\rho),\rho]) & (1.90)\end{aligned}$$

But if the Hamiltonian does not include the time-dependent perturbation(external field), $[h(\rho),\rho]$ will be zero because $|\Phi(t)\rangle \to |\Phi\rangle$ or $\rho(\boldsymbol{r};t) \to \rho(\boldsymbol{r})$.

Here we add the external field to the Hamiltonian as a perturbation.

$$\hat{H} \to \hat{H} + \hat{F}(t)$$

where

$$\hat{F}(t) = \sum_{kk'} f_{kk'}(t)c_k^\dagger c_{k'} = \int d\boldsymbol{r}\psi^\dagger(\boldsymbol{r})f(\boldsymbol{r};t)\psi(\boldsymbol{r})$$

Hence

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\rho(\boldsymbol{r};t) &= \langle\Phi(t)|\left[\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}), \hat{H}+\hat{F}(t)\right]|\Phi(t)\rangle & (1.91)\\ &= \int d\boldsymbol{r}' \left(h(\boldsymbol{r}\boldsymbol{r}')\rho(\boldsymbol{r}',\boldsymbol{r};t) - \rho(\boldsymbol{r},\boldsymbol{r}';t)h(\boldsymbol{r}'\boldsymbol{r})\right) + [f(\boldsymbol{r};t),\rho(\boldsymbol{r})] & \\ &\quad (= [h(\rho)+f(t),\rho]) & (1.92)\end{aligned}$$

This is so-called "*Time-dependent Hartree-Fock equation*"

1.6.1 Linear responce equation

If the unperturbed gorund state of the nucleus has a density matrix ρ_0, the time-dependent one can be expanded as

$$\rho(t) = \rho_0 + \delta\rho(t) \tag{1.93}$$

The mean field hamiltonian can be also expanded as

$$h(\rho) = h(\rho_0 + \delta\rho(t)) \approx h(\rho_0) + \frac{\delta h(\rho)}{\delta\rho}|_{\rho=\rho_0}\delta\rho(t) \tag{1.94}$$

Substituting these expansion to the time-dependent Hartree-Fock equation, we can obtain

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\delta\rho(t) &= \left[h(\rho_0) + \frac{\delta h(\rho)}{\delta\rho}|_{\rho=\rho_0}\delta\rho(t) + f(t), \rho_0 + \delta\rho(t)\right] & \\ &\approx [h(\rho_0),\delta\rho(t)] + \left[\frac{\delta h(\rho)}{\delta\rho}|_{\rho=\rho_0}\delta\rho(t), \rho_0\right] + [f(t),\rho_0] & (1.95)\end{aligned}$$

Using The Fourier transformation, (1.95) becomes

$$\hbar\omega\delta\rho(\omega) \approx [h(\rho_0),\delta\rho(\omega)] + \left[\frac{\delta h(\rho)}{\delta\rho}|_{\rho=\rho_0}\delta\rho(\omega) + f(\omega), \rho_0\right] \tag{1.96}$$

The explicit coordinate representation is

$$\begin{aligned} \hbar\omega\delta\rho(\boldsymbol{r};\omega) \approx & \int d\boldsymbol{r}' \left[h(\boldsymbol{r}\boldsymbol{r}')\delta\rho(\boldsymbol{r}'\boldsymbol{r};\omega) - \delta\rho(\boldsymbol{r}\boldsymbol{r}';\omega)h(\boldsymbol{r}'\boldsymbol{r})\right] \\ & + \int d\boldsymbol{r}' \iint d\boldsymbol{r}_1 d\boldsymbol{r}_2 \left[\frac{\delta h(\boldsymbol{r}\boldsymbol{r}')}{\delta\rho(\boldsymbol{r}_1\boldsymbol{r}_2)}|_{\rho=\rho_0}\delta\rho(\boldsymbol{r}_1\boldsymbol{r}_2;\omega)\rho_0(\boldsymbol{r}'\boldsymbol{r}) - \rho_0(\boldsymbol{r}\boldsymbol{r}')\frac{\delta h(\boldsymbol{r}'\boldsymbol{r})}{\delta\rho(\boldsymbol{r}_1\boldsymbol{r}_2)}|_{\rho=\rho_0}\delta\rho(\boldsymbol{r}_1\boldsymbol{r}_2;\omega)\right] \\ & + [f(\boldsymbol{r};\omega),\rho_0(\boldsymbol{r})] \end{aligned} \tag{1.97}$$

1.6.2 Time dependent perturbation theory

The time-dependent single particle wave function

$$\begin{aligned}\phi_k(\boldsymbol{r}(t)) &= \langle \boldsymbol{r}:t|k\rangle = \langle -|\psi(\boldsymbol{r}t)|k\rangle \\ &= \langle -|\hat{\mathrm{U}}^\dagger(t)\psi(\boldsymbol{r})\hat{\mathrm{U}}(t)|k\rangle\end{aligned}$$

where $\hat{\mathrm{U}}(t)$ is the time evolution operator, which is given by

$$\hat{\mathrm{U}}(t) \equiv e^{-\frac{i}{\hbar}(t-t_0)\hat{h}_0} \qquad (\ \hat{h}_0|k\rangle = \pm\epsilon_k|k\rangle \quad \hat{h}_0|-\rangle = 0\ )$$

Then the single particle wave function satisfies

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}\phi_k(\boldsymbol{r}(t)) &= \langle -|\hat{\mathrm{U}}^\dagger(t)\left[\psi(\boldsymbol{r}),\hat{h}_0\right]\hat{\mathrm{U}}(t)|k\rangle \\ &= \iint d\boldsymbol{r}_1 d\boldsymbol{r}_2 h(\boldsymbol{r}_1\boldsymbol{r}_2)\langle -|\hat{\mathrm{U}}^\dagger(t)\left[\psi(\boldsymbol{r}),\psi^\dagger(\boldsymbol{r}_1)\psi(\boldsymbol{r}_2)\right]\hat{\mathrm{U}}(t)|k\rangle \\ &= \int d\boldsymbol{r}' h(\boldsymbol{r}\boldsymbol{r}')\langle -|\hat{\mathrm{U}}^\dagger(t)\psi(\boldsymbol{r}')\hat{\mathrm{U}}(t)|k\rangle = \pm\epsilon_k\phi_k(\boldsymbol{r}(t))\end{aligned}$$

This is the time-dependent Hartree-Fock equation for the single particle wave function without the time-dependent external field. The solution of this equation is given by

$$\phi_k(\boldsymbol{r}(t)) = e^{\mp\frac{i}{\hbar}\epsilon_k(t-t_0)}\phi_k(\boldsymbol{r})$$

The additional weak external field is a perturbation, and changes the time-dependent wave function and the mean field.

$$\begin{aligned}\phi_k(\boldsymbol{r}(t)) = e^{\mp\frac{i}{\hbar}\epsilon_k(t-t_0)}\phi_k(\boldsymbol{r}) &\rightarrow e^{\mp\frac{i}{\hbar}\epsilon_k(t-t_0)}\left(\phi_k(\boldsymbol{r}) + \delta\phi_k(\boldsymbol{r}t)\right) \\ h(\boldsymbol{r}\boldsymbol{r}') &\rightarrow h(\boldsymbol{r}\boldsymbol{r}') + \frac{\delta h}{\delta\rho}(\boldsymbol{r}\boldsymbol{r}':t) + f(\boldsymbol{r}t)\end{aligned}$$

Thus the time-dependent HF equation becomes

$$\pm\epsilon_k\delta\phi_k(\boldsymbol{r}t) + i\hbar\frac{\partial}{\partial t}\delta\phi_k(\boldsymbol{r}t) = \int d\boldsymbol{r}'\left(h(\boldsymbol{r}\boldsymbol{r}')\delta\phi_k(\boldsymbol{r}'t) + \frac{\delta h}{\delta\rho}(\boldsymbol{r}\boldsymbol{r}':t)\phi_k(\boldsymbol{r}')\right) + f(\boldsymbol{r}t)\phi_k(\boldsymbol{r})$$

By the Fourier transformation, this equation can be rewritten.

$$\delta\phi_k(\boldsymbol{r}t) = \frac{1}{2\pi}\int d\omega e^{-i\omega t}\delta\phi_k(\boldsymbol{r}\omega) \qquad f(\boldsymbol{r}t) = \frac{1}{2\pi}\int d\omega e^{-i\omega t}f(\boldsymbol{r}\omega)$$

Thus

$$\int d\boldsymbol{r}' h(\boldsymbol{r}\boldsymbol{r}')\delta\phi_k(\boldsymbol{r}'\omega) - (\hbar\omega \pm \epsilon_k)\,\delta\phi_k(\boldsymbol{r}\omega) = -\int d\boldsymbol{r}'\frac{\delta h}{\delta\rho}(\boldsymbol{r}\boldsymbol{r}':\omega)\phi_k(\boldsymbol{r}') - f(\boldsymbol{r}\omega)\phi_k(\boldsymbol{r})$$

If we use the delta-type interaction in the Hartree-Fock mean field like as the Skyrme interaction, this equation takes the form as

$$\left(-\nabla\frac{\hbar^2}{2m^*(\boldsymbol{r})}\cdot\nabla + U(\boldsymbol{r}) - \hbar\omega \mp \epsilon_k\right)\delta\phi_k(\boldsymbol{r}\omega) = -\left(\frac{\delta h}{\delta\rho}(\boldsymbol{r}:\omega) + f(\boldsymbol{r}\omega)\right)\phi_k(\boldsymbol{r}) \qquad (1.98)$$

This type equation is so-called "*Sturm-Liouville equation*", and the solution is given by using the Green function.

$$\delta\phi_k(\boldsymbol{r}\omega) = \int d\boldsymbol{r}' G_0(\boldsymbol{r}\boldsymbol{r}':\hbar\omega \pm \epsilon_k + i\eta)\left(\frac{\delta h}{\delta\rho}(\boldsymbol{r}':\omega) + f(\boldsymbol{r}'\omega)\right)\phi_k(\boldsymbol{r}') \qquad (1.99)$$

The Green function is defined as

$$\left(-\nabla\frac{\hbar^2}{2m^*(\boldsymbol{r})}\cdot\nabla + U(\boldsymbol{r}) - E\right)G_0(\boldsymbol{r}\boldsymbol{r}':E) = -\delta(\boldsymbol{r}-\boldsymbol{r}')$$

The spectral representation of the green function

If one expands the HF green function in terms of ϕ_i as

$$G_0(\boldsymbol{r},\boldsymbol{r}';E) = \sum_{i\in all} \left(\phi_i(\boldsymbol{r})C_i(\boldsymbol{r}')\right) \tag{1.100}$$

one can get

$$\begin{aligned}\left(\hat{h}_0(\boldsymbol{r}) - E\right) G_0(\boldsymbol{r},\boldsymbol{r}';E) &= -\sum_{i\in all} \left((E-\epsilon_i)\phi_i(\boldsymbol{r})C_i(\boldsymbol{r}')\right) \\ &= -\delta(\boldsymbol{r}-\boldsymbol{r}')\end{aligned} \tag{1.101}$$

By using of the orthonormality of the wave function, one can obtain C.

$$C_i(\boldsymbol{r}') = \frac{\phi_i^*(\boldsymbol{r}')}{E-\epsilon_i} \tag{1.102}$$

So the HF green function can be expressed as

$$G_0(\boldsymbol{r},\boldsymbol{r}';E) = \sum_{i\in all} \left(\frac{\phi_i(\boldsymbol{r})\phi_i^*(\boldsymbol{r}')}{E-\epsilon_i}\right) \tag{1.103}$$

1.6.3 Energy weighted sum rule

The energy weighted sum rule S_1 can be written as a double commutator

$$S_1 = \sum_\nu (E_\nu - E_0)\,|\langle\nu|\hat{F}|0\rangle|^2 = \frac{1}{2}\langle 0|\left[\hat{F},\left[\hat{H},\hat{F}\right]\right]|0\rangle$$

This double commutator can be expressed in the configuration space as where we put the Hamiltonian and the external field

$$\begin{aligned}\left[\hat{F},\left[\hat{H},\hat{F}\right]\right] &= \sum_{ij} f_{ij} \sum_{kl} h_{kl} \sum_{mn} f_{mn} \left[c_i^\dagger c_j, \left[c_k^\dagger c_l, c_m^\dagger c_n\right]\right] \\
&= \sum_{ij} f_{ij} \sum_{kl} h_{kl} \sum_{mn} f_{mn} \left[c_i^\dagger c_j, \left[\delta_{lm} c_k^\dagger c_n - \delta_{kn} c_m^\dagger c_l\right]\right] \\
&= \sum_{ij} f_{ij} \sum_{kl} h_{kl} \sum_{mn} f_{mn} \left\{\delta_{lm}\left(\delta_{jk} c_i^\dagger c_n - \delta_{in} c_k^\dagger c_j\right) - \delta_{kn}\left(\delta_{jm} c_i^\dagger c_l - \delta_{il} c_m^\dagger c_j\right)\right\} \\
&= \sum_{ij}\sum_{ln} f_{ij} h_{jl} f_{ln} c_i^\dagger c_n - \sum_{ij}\sum_{kl} h_{kl} f_{li} f_{ij} c_k^\dagger c_j - \sum_{ij}\sum_{kl} f_{ij} f_{jk} h_{kl} c_i^\dagger c_l + \sum_{ij}\sum_{km} f_{mk} h_{ki} f_{ij} c_m^\dagger c_j \\
&= \sum_{ij}\sum_{kl} \left(f_{kj} h_{ji} f_{il} - h_{kj} f_{ji} f_{il} - f_{kj} f_{ji} h_{il} + f_{kj} h_{ji} f_{il}\right) c_k^\dagger c_l\end{aligned}$$

where $\quad [AB,CD] = \{B,C\}AD - \{B,D\}AC + \{A,C\}DB - \{A,D\}CB$

$$\langle 0|c_i^\dagger c_j|0\rangle = \overline{c_i^\dagger c_j} = \theta(k_F - k_i)\delta_{ij}$$

$$\hat{H} = \sum_{ij} h_{ij} c_i^\dagger c_j \qquad \hat{F} = \sum_{ij} f_{ij} c_i^\dagger c_j$$

Thus

$$\langle 0|\left[\hat{F},\left[\hat{H},\hat{F}\right]\right]|0\rangle = \sum_{ij}\sum_{k\in hole} \{2f_{kj}h_{ji}f_{ik} - h_{kj}f_{ji}f_{ik} - f_{kj}f_{ji}h_{ik}\}$$

Also in the coordinate space,

$$\begin{aligned}\left[\hat{F},\left[\hat{H},\hat{F}\right]\right] &= \iiiint d\boldsymbol{r}d\boldsymbol{r}'d\boldsymbol{r}_1 d\boldsymbol{r}_2 f(\boldsymbol{r})f(\boldsymbol{r}')h(\boldsymbol{r}_1\boldsymbol{r}_2)\left[\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}),\left[\psi^\dagger(\boldsymbol{r}_1)\psi(\boldsymbol{r}_2),\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r}')\right]\right] \\
&= \iiiint d\boldsymbol{r}d\boldsymbol{r}'d\boldsymbol{r}_1 d\boldsymbol{r}_2 f(\boldsymbol{r})f(\boldsymbol{r}')h(\boldsymbol{r}_1\boldsymbol{r}_2)\end{aligned}$$

$$\times \left[\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}), \left[\delta(\boldsymbol{r}'-\boldsymbol{r}_2)\psi^\dagger(\boldsymbol{r}_1)\psi(\boldsymbol{r}') - \delta(\boldsymbol{r}'-\boldsymbol{r}_1)\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r}_2)\right]\right]$$

$$= \iiiint d\boldsymbol{r}d\boldsymbol{r}'d\boldsymbol{r}_1 d\boldsymbol{r}_2 f(\boldsymbol{r})f(\boldsymbol{r}')h(\boldsymbol{r}_1\boldsymbol{r}_2)$$

$$\times\Big[\delta(\boldsymbol{r}'-\boldsymbol{r}_2)\left(\delta(\boldsymbol{r}-\boldsymbol{r}_1)\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}') - \delta(\boldsymbol{r}-\boldsymbol{r}')\psi^\dagger(\boldsymbol{r}_1)\psi(\boldsymbol{r})\right)$$

$$-\delta(\boldsymbol{r}'-\boldsymbol{r}_1)\left(\delta(\boldsymbol{r}-\boldsymbol{r}')\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}_2) - \delta(\boldsymbol{r}-\boldsymbol{r}_2)\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r})\right)\Big]$$

$$= \iint d\boldsymbol{r}d\boldsymbol{r}'\left(2\psi^\dagger(\boldsymbol{r})f(\boldsymbol{r})h(\boldsymbol{r}\boldsymbol{r}')f(\boldsymbol{r}')\psi(\boldsymbol{r}') - \psi^\dagger(\boldsymbol{r})h(\boldsymbol{r}\boldsymbol{r}')f^2(\boldsymbol{r}')\psi(\boldsymbol{r}') - \psi^\dagger(\boldsymbol{r})f^2(\boldsymbol{r})h(\boldsymbol{r}\boldsymbol{r}')\psi(\boldsymbol{r}')\right)$$

Thus

$$\langle 0|\left[\hat{F},\left[\hat{H},\hat{F}\right]\right]|0\rangle = \iint d\boldsymbol{r}d\boldsymbol{r}'\left(2f(\boldsymbol{r})f(\boldsymbol{r}')h(\boldsymbol{r}\boldsymbol{r}')\rho(\boldsymbol{r}'\boldsymbol{r}) - h(\boldsymbol{r}\boldsymbol{r}')f^2(\boldsymbol{r}')\rho(\boldsymbol{r}'\boldsymbol{r}) - f^2(\boldsymbol{r})h(\boldsymbol{r}\boldsymbol{r}')\rho(\boldsymbol{r}'\boldsymbol{r})\right)$$

where we put the Hamiltonian and the external field

$$\hat{H} = \iint d\boldsymbol{r}_1 d\boldsymbol{r}_2 h(\boldsymbol{r}_1\boldsymbol{r}_2)\psi^\dagger(\boldsymbol{r}_1)\psi(\boldsymbol{r}_2) \qquad \hat{F} = \int d\boldsymbol{r} f(\boldsymbol{r})\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r})$$

For the most simple example, we put

$$h(\boldsymbol{r}\boldsymbol{r}') \to \frac{-\hbar^2}{2m}\nabla^2\delta(\boldsymbol{r}-\boldsymbol{r}') + U(\boldsymbol{r})\delta(\boldsymbol{r}-\boldsymbol{r}') \qquad \text{No velosity terms in the potential}$$

Then

$$\langle 0|\left[\hat{F},\left[\hat{H},\hat{F}\right]\right]|0\rangle = \int d\boldsymbol{r}\frac{\hbar^2}{m}\left(\nabla f(\boldsymbol{r})\right)^2\rho(\boldsymbol{r}) = \sum_i \int d\boldsymbol{r}\frac{\hbar^2}{m}\phi_i^*(\boldsymbol{r})\left[\nabla f(\boldsymbol{r})\right]^2\phi_i(\boldsymbol{r})$$

$$= \frac{\hbar^2}{m}\langle[\nabla f]^2\rangle$$

Next example is the Hamiltonian which is contained the effective mass.

$$h(\boldsymbol{r}\boldsymbol{r}') \to \nabla\cdot\frac{-\hbar^2}{2m^*(\boldsymbol{r})}\nabla\delta(\boldsymbol{r}-\boldsymbol{r}') + U(\boldsymbol{r})\delta(\boldsymbol{r}-\boldsymbol{r}')$$

Also in this case,

$$\langle 0|\left[\hat{F},\left[\hat{H},\hat{F}\right]\right]|0\rangle = \int d\boldsymbol{r}\frac{\hbar^2}{m^*(\boldsymbol{r})}\left(\nabla f(\boldsymbol{r})\right)^2\rho(\boldsymbol{r}) = \sum_i \int d\boldsymbol{r}\phi_i^*(\boldsymbol{r})\frac{\hbar^2}{m^*(\boldsymbol{r})}\left[\nabla f(\boldsymbol{r})\right]^2\phi_i(\boldsymbol{r})$$

$$= \langle\frac{\hbar^2}{m^*}\left[\nabla f\right]^2\rangle$$

Example : Sum rule for the multipole operator

For the multipole operator, $f = \sum_\mu r^\lambda Y_{\lambda\mu}$, by using the gradient formula[(6-171),B.M.vol.I,p401],

$$\sum_\mu \nabla\phi(r)Y_{\lambda\mu}^*\cdot\nabla\phi(r)Y_{\lambda\mu} = \frac{2\lambda+1}{4\pi}\left(\left(\frac{\mathrm{d}\phi}{\mathrm{d}r}\right)^2 + \lambda(\lambda+1)\left(\frac{\phi}{r}\right)^2\right)$$

the gradient $(\nabla f)^2$ becomes

$$\sum_\mu |\nabla r^\lambda Y_{\lambda\mu}|^2 = \frac{\lambda(2\lambda+1)^2}{4\pi}r^{2\lambda-2}$$

Then

$$\langle(\nabla f)^2\rangle = \sum_{i\sigma}\int d\boldsymbol{r}\phi_i^*(\boldsymbol{r}\sigma)\sum_\mu\left(\nabla r^\lambda Y_{\lambda\mu}\right)^2\phi_i(\boldsymbol{r}\sigma) = \frac{\lambda(2\lambda+1)^2}{4\pi}\sum_{nlj}\int dr\phi_{nlj}(r)r^{2\lambda-2}\phi_{nlj}(r)$$

$$= \frac{\lambda(2\lambda+1)^2}{4\pi}\langle r^{2\lambda-2}\rangle$$

$$\phi_i(\boldsymbol{r}\sigma) = \mathcal{Y}_{ljm}\frac{\phi_{lj}(r,E_n)}{r} \qquad \mathcal{Y}_{ljm}(\tilde{\boldsymbol{r}}\sigma) = \sum_{m_l s}\langle lm_l;\frac{1}{2}s|jm\rangle Y_{lm_l}\chi_s(\sigma)$$

Thus one can get the Thomas-Reiche-Kuhn sum rule

$$S_1 = \frac{\hbar^2}{2m}\frac{\lambda(2\lambda+1)}{4\pi}(2\lambda+1)\langle r^{2\lambda-2}\rangle$$

Chapter 2

Multipole field

2.1 Charge density

We have already studied the density operator. In addition, here we will study the charge density operator.

The charge density operator is defined by

$$\hat{\rho}_e(\boldsymbol{r}) \equiv \sum_{i=1}^{A} e\left(\frac{1}{2} - t_3(i)\right)\delta(\boldsymbol{r} - \hat{\boldsymbol{r}}_i) \tag{2.1}$$

$$\text{where} \qquad \left(\frac{1}{2} - t_3\right)|n\rangle = 0 \qquad \left(\frac{1}{2} - t_3\right)|p\rangle = 1$$

For the Slater determinant, the charge density operator satisfies

$$\begin{aligned}
\langle\Phi|\hat{\rho}_e(\boldsymbol{r})|\Phi\rangle &= \langle\Phi|\left[\sum_{i=1}^{A} e\left(\frac{1}{2} - t_3(i)\right)\delta(\boldsymbol{r} - \hat{\boldsymbol{r}}_i)\right]|\Phi\rangle \\
&= \int\!\!\cdots\!\!\int d\boldsymbol{r}_1 \ldots d\boldsymbol{r}_A \Phi^*_{\{k_1\ldots k_A\}}(\boldsymbol{r}_1 \ldots \boldsymbol{r}_A)\left[\sum_{i=1}^{A} e\left(\frac{1}{2} - t_3(i)\right)\delta(\boldsymbol{r} - \hat{\boldsymbol{r}}_i)\right]\Phi_{\{k_1\ldots k_A\}}(\boldsymbol{r}_1 \ldots \boldsymbol{r}_A) \\
&= \int\!\!\cdots\!\!\int d\boldsymbol{r}_1 \ldots d\boldsymbol{r}_Z \Phi^*_{\{k_1\ldots k_Z\}}(\boldsymbol{r}_1 \ldots \boldsymbol{r}_Z)\left[\sum_{i=1}^{Z} e\delta(\boldsymbol{r} - \hat{\boldsymbol{r}}_i)\right]\Phi_{\{k_1\ldots k_Z\}}(\boldsymbol{r}_1 \ldots \boldsymbol{r}_Z) \\
&= \sum_{i=1}^{Z} e\,|\phi_{p,k_i}(\boldsymbol{r})|^2 = \rho_p(\boldsymbol{r})
\end{aligned} \tag{2.2}$$

where $A = Z + N$ Z is the proton number and N is the neutron number.

2nd quantized charge density can be expressed as

$$\hat{\rho}_e(\boldsymbol{r}) \equiv \sum_{ij}\sum_{\tau}\int d\boldsymbol{r}'\phi_i^\dagger(\boldsymbol{r}'\tau)e\left(\frac{1}{2} - t_3\right)\delta(\boldsymbol{r} - \hat{\boldsymbol{r}}')\phi_i(\boldsymbol{r}'\tau)c_i^\dagger c_i \tag{2.3}$$

$$= e\psi_p^\dagger(\boldsymbol{r})\psi_p(\boldsymbol{r}) \tag{2.4}$$

2.1.1 The multipole expansion of the electro-magnetic field

The interaction Hamiltonian between the electro-magnetic external field and the nucleus is given by

$$\begin{aligned}
H_{int} &= -\frac{1}{c}\int d^3\boldsymbol{r} j_\mu A^\mu = \int d^3\boldsymbol{r}\left(\rho(\boldsymbol{r},t)\Phi(\boldsymbol{r},t) - \frac{1}{c}\boldsymbol{j}(\boldsymbol{r},t)\cdot\boldsymbol{A}(\boldsymbol{r},t)\right) \\
&= \int d^3\boldsymbol{r}\left(\rho(\boldsymbol{r},t)\Phi(\boldsymbol{r},t) - \boldsymbol{\mu}(\boldsymbol{r},t)\cdot\boldsymbol{B}(\boldsymbol{r},t)\right)
\end{aligned}$$

where $\boldsymbol{\mu}$ is the magnetic moment and $\boldsymbol{B}$ is the magnetic flux density, which are defined by

$$\boldsymbol{j}(\boldsymbol{r},t) \equiv c\nabla \times \boldsymbol{\mu}(\boldsymbol{r},t) \qquad \boldsymbol{B}(\boldsymbol{r},t) \equiv \nabla \times \boldsymbol{A}(\boldsymbol{r},t)$$

If the sorces are far from the nucleus, and the quantities ϕ and $\boldsymbol{B}$ are static, these quantities satisfies the homogeneous Maxwell equations,

$$\Delta\Phi(\boldsymbol{r}) = 0 \qquad \nabla\times\boldsymbol{B}(\boldsymbol{r}) = \boldsymbol{0} \qquad \nabla\cdot\boldsymbol{B}(\boldsymbol{r}) = 0$$

This means that $\boldsymbol{B}$ can be written as

$$\boldsymbol{B}(\boldsymbol{r}) = -\nabla\Xi \qquad \text{with} \qquad \Delta\Xi(\boldsymbol{r}) = 0$$

The general solution of the Laplace equation is given by

$$f(\boldsymbol{r}) = \sum_{\lambda\mu} a_{\lambda\mu} r^\lambda Y_{\lambda\mu}(\hat{\boldsymbol{r}}) \qquad \text{with} \qquad \Delta f(\boldsymbol{r}) = \left(\frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{\boldsymbol{l}^2}{r^2}\right) f(\boldsymbol{r}) = 0 \qquad \text{(Laplace equation)}$$

Then the Hamiltonian can be rewritten as

$$\begin{aligned} H_{int} &= \sum_{\lambda\mu}\left\{a_{\lambda\mu}\left(\int d\boldsymbol{r}\rho(\boldsymbol{r})r^\lambda Y_{\lambda\mu}(\hat{\boldsymbol{r}})\right) + b_{\lambda\mu}\left(\int d\boldsymbol{r}\boldsymbol{\mu}(\boldsymbol{r})\cdot\nabla\left(r^\lambda Y_{\lambda\mu}(\hat{\boldsymbol{r}})\right)\right)\right\} \\ &= \sum_{\lambda\mu}\left\{a_{\lambda\mu}\left(\int d\boldsymbol{r}\rho(\boldsymbol{r})r^\lambda Y_{\lambda\mu}(\hat{\boldsymbol{r}})\right) + b_{\lambda\mu}\left(\int d\boldsymbol{r}\left(\boldsymbol{\mu}_l(\boldsymbol{r}) + \boldsymbol{\mu}_s(\boldsymbol{r})\right)\cdot\nabla\left(r^\lambda Y_{\lambda\mu}(\hat{\boldsymbol{r}})\right)\right)\right\} \end{aligned}$$

2.1.2 Isovector, Isoscalar operator

1st Quantized representation

$$\begin{aligned} \hat{Q}^\lambda_{IV} &= \sum_{i=1}^{A}\sum_{\mu}\hat{\tau}_3(i)r^\lambda(i)Y_{\lambda\mu}(i), & \hat{Q}^\lambda_{IS} &= \sum_{i=1}^{A}\sum_{\mu} r^\lambda(i)Y_{\lambda\mu}(i) \\ &= \hat{Q}^\lambda_n - \hat{Q}^\lambda_p & &= \hat{Q}^\lambda_n + \hat{Q}^\lambda_p \end{aligned}$$

2nd Quantized representation

$$\begin{aligned} \hat{Q}^\lambda_{IV} &= \sum_{i,j}\sum_{q,\mu}\int d\boldsymbol{r}\phi^*_{q,i}(\boldsymbol{r})\hat{\tau}_3 r^\lambda Y_{\lambda\mu}\phi_{q,j}(\boldsymbol{r})c^\dagger_i c_j, & \hat{Q}^\lambda_{IS} &= \sum_{i,j}\sum_{\mu,q}\int d\boldsymbol{r}\phi^*_{q,i}(\boldsymbol{r})r^\lambda Y_{\lambda\mu}\phi_{q,j}(\boldsymbol{r})c^\dagger_i c_j, \\ &= \sum_{\mu,q}\int d\boldsymbol{r}\hat{\psi}^*_q(\boldsymbol{r})\hat{\tau}_3 r^\lambda Y_{\lambda\mu}\hat{\psi}_q(\boldsymbol{r}), & &= \sum_{\mu,q}\int d\boldsymbol{r}\hat{\psi}^*_q(\boldsymbol{r})r^\lambda Y_{\lambda\mu}\hat{\psi}_q(\boldsymbol{r}), \\ &= \hat{Q}^\lambda_n - \hat{Q}^\lambda_p & &= \hat{Q}^\lambda_n + \hat{Q}^\lambda_p \end{aligned}$$

Note that

$$\hat{t}_3 = \frac{1}{2}\hat{\tau}_3 \qquad \hat{\tau}_3|n\rangle = |n\rangle \qquad \hat{\tau}_3|p\rangle = -|p\rangle$$

2.1.3 E1 operator(Mass Center removed Isovector Dipole operator)

$$\begin{aligned} \hat{Q}_{E1} &= e\sum_{\mu=-1}^{+1}\sum_{i=1}^{A}\frac{1}{2}\left(1-\hat{\tau}_3(i)\right)r(i)Y_{1\mu}(i) \\ &= e\sum_{\mu=-1}^{+1}\sum_{i=1}^{Z} r(i)Y_{1\mu}(i) = e\sum_{i=1}^{Z}\sqrt{\frac{3}{4\pi}}\sum_{\mu=-1}^{+1} r_\mu(i) = e\sum_{i=1}^{Z}\sqrt{\frac{3}{4\pi}}z(i) \end{aligned}$$

Note that

$$rY_{1\mu} = r_\mu : \qquad r_\pm = \mp\frac{1}{\sqrt{2}}(x \pm iy) \qquad r_0 = z$$

In terms of the Center of Mass system, the total linear momentum vanishes. In general, the coordinate of the center of mass system $\tilde{\boldsymbol{r}}$ is given by

$$\begin{aligned} \tilde{\boldsymbol{r}}_i = \boldsymbol{r}_i - \boldsymbol{R} &= \boldsymbol{r}_i - \frac{1}{A}\sum_{j=1}^{A}\boldsymbol{r}_j = \boldsymbol{r}_i - \frac{1}{A}\sum_{j=1}^{Z}\boldsymbol{r}_j - \frac{1}{A}\sum_{j=1}^{N}\boldsymbol{r}_j \\ &= \boldsymbol{r}_i - \frac{Z}{A}\boldsymbol{R}_p - \frac{N}{A}\boldsymbol{R}_n \end{aligned}$$

then one can get the center-mass removed E1 operator by replacing $r_\mu \to \tilde{r}_\mu$

$$\begin{aligned}
\hat{Q}^{CM}_{E1} &= e\sqrt{\frac{3}{4\pi}} \sum_{\mu=-1}^{+1} \sum_{i=1}^{Z} \tilde{r}_\mu(i) \\
&= e\sqrt{\frac{3}{4\pi}} \sum_{\mu=-1}^{+1} \sum_{i=1}^{Z} \left(r_\mu(i) - \frac{N}{A} R^n_\mu - \frac{Z}{A} R^p_\mu \right) \\
&= e\sqrt{\frac{3}{4\pi}} \sum_{\mu=-1}^{+1} \left(Z R^p_\mu - \frac{ZN}{A} R^n_\mu - \frac{Z^2}{A} R^p_\mu \right) \\
&= e\sqrt{\frac{3}{4\pi}} \sum_{\mu=-1}^{+1} \frac{ZN}{A} \left(R^p_\mu - R^n_\mu \right) = e\sqrt{\frac{3}{4\pi}} \frac{ZN}{A} \left(\frac{1}{Z} \sum_{i=1}^{Z} z_p(i) - \frac{1}{N} \sum_{i=1}^{N} z_n(i) \right) \\
&= e\frac{ZN}{A} \sum_{\mu} \left(\frac{1}{Z} \sum_{i=1}^{Z} r(i) Y_{1\mu}(i) - \frac{1}{N} \sum_{i=1}^{N} r(i) Y_{1\mu} \right) \\
&= -e \sum_{\mu} \sum_{i=1}^{A} \hat{t}_3(i) \left(r(i) Y_{1\mu}(i) - \frac{1}{A} \sum_{j=1}^{A} r(j) Y_{1\mu}(j) \right)
\end{aligned}$$

Chapter 3

Random Phase approximation

3.1 Liner responce theory

3.2 Derivation of the unperturbed responce function

The formal expression of the unperturbed responce function is given by

$$\begin{aligned} R_0(\boldsymbol{r}t, \boldsymbol{r}'t') &= -i\theta(t-t')\langle 0| \left[\hat{U}_0^\dagger(t)\hat{\rho}(\boldsymbol{r})\hat{U}_0(t), \hat{U}_0^\dagger(t')\hat{\rho}(\boldsymbol{r}')\hat{U}_0(t')\right]|0\rangle \\ &= -i\theta(t-t')\sum_{mi}\Big[\langle 0|\hat{U}_0^\dagger(t)\hat{\rho}(\boldsymbol{r})\hat{U}_0(t)|mi\rangle\langle mi|\hat{U}_0^\dagger(t')\hat{\rho}(\boldsymbol{r}')\hat{U}_0(t')|0\rangle \\ &\qquad -\langle 0|\hat{U}_0^\dagger(t')\hat{\rho}(\boldsymbol{r}')\hat{U}_0(t')|mi\rangle\langle mi|\hat{U}_0^\dagger(t)\hat{\rho}(\boldsymbol{r})\hat{U}_0(t)|0\rangle\Big] \\ &= -i\theta(t-t')\sum_{mi}\Big[e^{-i(t-t')(\epsilon_m-\epsilon_i)/\hbar}\langle 0|\hat{\rho}(\boldsymbol{r})|mi\rangle\langle mi|\hat{\rho}(\boldsymbol{r}')|0\rangle \\ &\qquad -e^{i(t-t')(\epsilon_m-\epsilon_i)/\hbar}\langle 0|\hat{\rho}(\boldsymbol{r}')|mi\rangle\langle mi|\hat{\rho}(\boldsymbol{r})|0\rangle\Big] \end{aligned}$$

where $\hat{U}_0(t) = e^{-i(t-t_0)\hat{h}_0/\hbar}$, $|m\rangle$ is a particle state and $|i\rangle$ is a hole state.
Note that $\hat{h}_0$ is the mean field hamiltonian, which has properties as

$$\hat{h}_0|0\rangle = 0, \qquad \hat{h}_0|mi\rangle = \hat{h}_0 a_m^\dagger b_i^\dagger|0\rangle = (\epsilon_m - \epsilon_i)|mi\rangle$$
$$\hat{h}_0 = \sum_m \epsilon_m a_m^\dagger a_m - \sum_i \epsilon_i b_i^\dagger b_i \qquad (m \in \text{particle} \quad i \in \text{hole})$$

Applying

$$\theta(t-t') = \frac{-1}{2\pi i}\int_{-\infty}^{\infty} d\tilde{\omega}\frac{e^{i\tilde{\omega}(t-t')}}{\tilde{\omega}-i\eta}\left(= \frac{-1}{2\pi i}\int_{-\infty}^{\infty} d\tilde{\omega}\frac{e^{-i\tilde{\omega}(t-t')}}{\tilde{\omega}+i\eta}\right) \tag{3.1}$$

to $R_0(\boldsymbol{r}t, \boldsymbol{r}'t')$, one can get

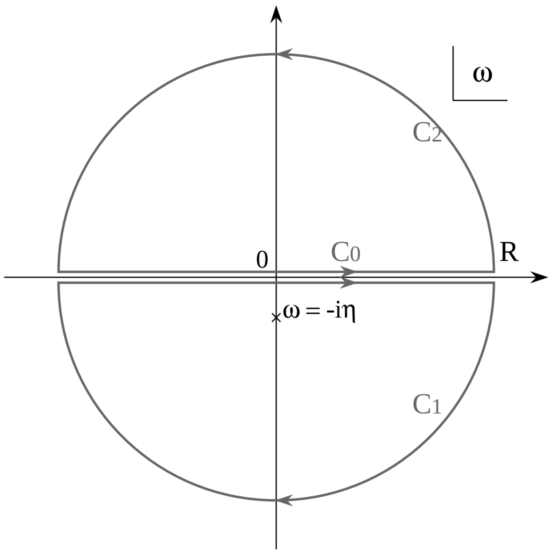
$$\begin{aligned} R_0(\boldsymbol{r}t, \boldsymbol{r}'t') &= \frac{1}{2\pi}\sum_{mi}\int_{-\infty}^{\infty} d\tilde{\omega}\frac{1}{\tilde{\omega}-i\eta}\Big[e^{i(t-t')(\tilde{\omega}-(\epsilon_m-\epsilon_i)/\hbar)}\langle 0|\hat{\rho}(\boldsymbol{r})|mi\rangle\langle mi|\hat{\rho}(\boldsymbol{r}')|0\rangle \\ &\qquad -e^{i(t-t')(\tilde{\omega}+(\epsilon_m-\epsilon_i)/\hbar)}\langle 0|\hat{\rho}(\boldsymbol{r}')|mi\rangle\langle mi|\hat{\rho}(\boldsymbol{r})|0\rangle\Big] \end{aligned}$$

Then, the Fourier transform of the unperturbed responce function can be obtained

$$
\begin{aligned}
R_0(\boldsymbol{r}\boldsymbol{r}',\omega) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} d(t-t')e^{i\omega(t-t')}R_0(\boldsymbol{r}t,\boldsymbol{r}'t') \\
&= \frac{1}{2\pi}\sum_{mi}\int_{-\infty}^{\infty} d\tilde{\omega}\Big[\frac{1}{\tilde{\omega}-i\eta}\delta(\tilde{\omega}+\omega-(\epsilon_m-\epsilon_i)/\hbar)\langle 0|\hat{\rho}(\boldsymbol{r})|mi\rangle\langle mi|\hat{\rho}(\boldsymbol{r}')|0\rangle \\
&\qquad -\frac{1}{\tilde{\omega}-i\eta}\delta(\tilde{\omega}+\omega+(\epsilon_m-\epsilon_i)/\hbar)\langle 0|\hat{\rho}(\boldsymbol{r}')|mi\rangle\langle mi|\hat{\rho}(\boldsymbol{r})|0\rangle\Big] \\
&= \frac{\hbar}{2\pi}\sum_{mi}\left[\frac{\langle 0|\hat{\rho}(\boldsymbol{r})|mi\rangle\langle mi|\hat{\rho}(\boldsymbol{r}')|0\rangle}{(\epsilon_m-\epsilon_i)-\hbar\omega-i\eta}+\frac{\langle 0|\hat{\rho}(\boldsymbol{r}')|mi\rangle\langle mi|\hat{\rho}(\boldsymbol{r})|0\rangle}{(\epsilon_m-\epsilon_i)+\hbar\omega+i\eta}\right]
\end{aligned}
$$

The proof of (3.1)

$$
\theta(t-t') = \frac{-1}{2\pi i}\int_{-\infty}^{\infty} d\omega\frac{e^{-i\omega(t-t')}}{\omega+i\eta}
$$



To show the proof of this relation for the step function, we think the contour integration(left figure). When $t-t'>0 (t-t'<0)$ one takes a path $C_0+C_1(C_0+C_2)$, because $e^{-i\omega(t-t')}$ converges on $C_1(C_2)$ plane at the limit $\omega\to\infty$, and also

$$
\int_{C_1(C_2)}\frac{d\omega}{2\pi i}\frac{e^{-i\omega(t-t')}}{\omega+i\eta}\Bigg|_{R\to\infty}\to 0.
$$

Then one can calculate by using the residue theorem,

$$
\begin{aligned}
\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}\frac{e^{-i\omega(t-t')}}{\omega+i\eta} &= \int_{C_0}\frac{d\omega}{2\pi i}\frac{e^{-i\omega(t-t')}}{\omega+i\eta} \\
&= \begin{cases} (t-t'>0) & \displaystyle\int_{C_0+C_1}\frac{d\omega}{2\pi i}\frac{e^{-i\omega(t-t')}}{\omega+i\eta}\Bigg|_{\eta\to 0}\to -1 \\ (t-t'<0) & \displaystyle\int_{C_0+C_2}\frac{d\omega}{2\pi i}\frac{e^{-i\omega(t-t')}}{\omega+i\eta}=0 \end{cases}
\end{aligned}
$$

3.3 Sum rule

The RPA responce function is given by

$$
R(\boldsymbol{r},\boldsymbol{r}':\omega) = \sum_{\nu>0}\left(\frac{\langle 0|\hat{\rho}(\boldsymbol{r})|\nu\rangle\langle\nu|\hat{\rho}(\boldsymbol{r}')|0\rangle}{\hbar\omega-(E_\nu-E_0)+i\epsilon}-\frac{\langle 0|\hat{\rho}(\boldsymbol{r}')|\nu\rangle\langle\nu|\hat{\rho}(\boldsymbol{r})|0\rangle}{\hbar\omega+(E_\nu-E_0)+i\epsilon}\right)
$$

where $|\nu\rangle$ is an excited state which satisfies $\hat{H}|\nu\rangle=(E_\nu-E_0)|\nu\rangle$. If one use the relation,

$$
\hat{F} = \int d\boldsymbol{r}f(\boldsymbol{r})\hat{\rho}(\boldsymbol{r})\left(=\int d\boldsymbol{r}f(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\right)
$$

and $1/(\omega+i\epsilon)=\mathrm{P}(1/\omega)-i\pi\delta(\omega)$, then one can get

$$
\begin{aligned}
R_F(\omega)\equiv\int\int d\boldsymbol{r}d\boldsymbol{r}'f(\boldsymbol{r})R(\boldsymbol{r},\boldsymbol{r}':\omega)f(\boldsymbol{r}') &= \sum_{\nu>0}\left(\frac{\langle 0|\hat{F}|\nu\rangle\langle\nu|\hat{F}|0\rangle}{\hbar\omega-(E_\nu-E_0)+i\epsilon}-\frac{\langle 0|\hat{F}|\nu\rangle\langle\nu|\hat{F}|0\rangle}{\hbar\omega+(E_\nu-E_0)+i\epsilon}\right) \\
&= \sum_{\nu>0}\langle 0|\hat{F}|\nu\rangle\langle\nu|\left[\frac{1}{\hbar\omega-(\hat{H}-E_0)+i\epsilon}-\frac{1}{\hbar\omega+(\hat{H}-E_0)+i\epsilon}\right]|\nu\rangle\langle\nu|\hat{F}|0\rangle \\
&= \sum_{\nu>0}\Bigg\{\mathrm{P}\left(\frac{1}{\hbar\omega-(E_\nu-E_0)}-\frac{1}{\hbar\omega+(E_\nu-E_0)}\right) \\
&\qquad -i\pi\left(\delta(\hbar\omega-(E_\nu-E_0))-\delta(\hbar\omega+(E_\nu-E_0))\right)\Bigg\}|\langle\nu|\hat{F}|0\rangle|^2
\end{aligned}
$$

So one can get the relation for the positive frequency($\omega > 0$),

$$\text{Im}\int\int d\boldsymbol{r}d\boldsymbol{r}' f(\boldsymbol{r})R(\boldsymbol{r},\boldsymbol{r}':\omega)f(\boldsymbol{r}') = -\pi\sum_{\nu>0}\delta(\hbar\omega-(E_\nu-E_0))|\langle\nu|\hat{F}|0\rangle|^2$$

One can get the energy-weighted sum rule by integrating this relation,

$$S_1 = -\frac{\hbar^2}{\pi}\int_0^\infty d\omega\omega\text{Im}\int\int d\boldsymbol{r}d\boldsymbol{r}' f(\boldsymbol{r})R(\boldsymbol{r},\boldsymbol{r}':\omega)f(\boldsymbol{r}') = \sum_{\nu>0}(E_\nu-E_0)|\langle\nu|\hat{F}|0\rangle|^2$$

In general, a sum rule S_k is given by

$$S_k = \sum_\nu (E_\nu - E_0)^k|\langle\nu|F|0\rangle|^2 = \langle 0|F(H-E_0)^kF|0\rangle$$

3.4 Static polarizability and Spurious solution

When we think next Hamiltonian

$$H = H_0 + \lambda F \qquad (H_0 \text{ is the exact hamiltonian, or HF hamiltonian etc.})$$

here, F is the external field. The external field, can be expressed by the one body operator, can commute with H.

$$[H,F] = 0$$

For a state $|\lambda\rangle = e^{i\lambda F}|0\rangle$, the expectation value of the hamiltonian $\langle\lambda|H|\lambda\rangle$ can be expanded by λ as

$$\begin{aligned}\langle\lambda|H|\lambda\rangle &= \langle 0|H + i\lambda[H,F] + \frac{\lambda^2}{2}[[H,F],F] + \ldots|0\rangle \\ &= \langle 0|H|0\rangle\end{aligned}$$

$|\lambda\rangle$ is so-called 'the spurious state' which is caused by the spontaneously symmetry breaking in $|0\rangle$. Where $|0\rangle$ is the Hartree-Fock basis RPA ground state. The equation

$$\langle 0|[[H,F],F]|0\rangle = 0$$

can be expressed in matrix language as

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} F \\ -F^* \end{pmatrix} = 0$$

Also

$$\langle 0|[[H,F],F]|0\rangle =$$

3.5 RPA with Skyrme interaction

Skyrme Hartree-Fock equation is given as

$$
\begin{aligned}
& h_{0,q}[\rho]\phi_{q,i}(\boldsymbol{r}) = \epsilon_i \phi_{q,i}(\boldsymbol{r}) \\
& h_{0,q}[\rho]\phi_{q,i}(\boldsymbol{r}) \\
& \quad = -\left(\frac{\hbar^2}{2m} + B_3\rho(\boldsymbol{r}) + B_4\rho_q(\boldsymbol{r})\right)\Delta\phi_{q,i}(\boldsymbol{r}) + \left[B_3 2i\boldsymbol{j}(\boldsymbol{r}) + B_4 2i\boldsymbol{j}_q(\boldsymbol{r}) - B_3\nabla\rho(\boldsymbol{r}) - B_4\nabla\rho(\boldsymbol{r})\right]\cdot\nabla\phi_{q,i}(\boldsymbol{r}) \\
& \qquad + \left[2B_1\rho(\boldsymbol{r}) + (\alpha+2)B_7\rho^{\alpha+1}(\boldsymbol{r}) + 2B_2\rho_q(\boldsymbol{r}) + \alpha B_8\rho^{\alpha-1}(\boldsymbol{r})\sum_{q'}\rho_{q'}^2(\boldsymbol{r}) + 2B_8\rho^{\alpha}(\boldsymbol{r})\rho_q(\boldsymbol{r})\right]\phi_{q,i}(\boldsymbol{r}) \\
& \qquad + \left[B_3\left(\tau(\boldsymbol{r}) + i\nabla\cdot\boldsymbol{j}(\boldsymbol{r})\right) + B_4\left(\tau_q(\boldsymbol{r}) + i\nabla\cdot\boldsymbol{j}_q(\boldsymbol{r})\right) + 2B_5\Delta\rho(\boldsymbol{r}) + 2B_6\Delta\rho_q(\boldsymbol{r})\right]\phi_{q,i}(\boldsymbol{r})
\end{aligned}
$$

Here we ignored spin-dependent terms, but time-odd velocity dependent terms are included. Random-Phase-Approximation in the density functional theory can be formulated from

$$
\begin{aligned}
h_q(t) &= h_{0,q}[\rho] + \left\{\left[v^{ext} + \sum_{q'}\frac{\delta h_{0,q}[\rho]}{\delta\rho_{q'}}\delta\rho_{q'}\right]e^{-i\omega t} + h.c.\right\} \\
\phi_{q,i}(\boldsymbol{r},t) &= e^{-i\frac{\epsilon_i}{\hbar}t}\left[\phi_{q,i}(\boldsymbol{r}) + \delta\phi_{q,i}^{(-)}(\boldsymbol{r})e^{-i\omega t} + \delta\phi_{q,i}^{(+)}(\boldsymbol{r})e^{+i\omega t}\right]
\end{aligned}
$$

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\phi_{q,i}(\boldsymbol{r},t) &= h_q(t)\phi_{q,i}(\boldsymbol{r},t) \\
&\downarrow \quad \text{in the first order approximation} \\
\left(\hbar\omega + \epsilon_i - h_{0,q}\right)\delta\phi_{q,i}^{(-)}(\boldsymbol{r}) &= \left[v^{ext} + \sum_{q'}\frac{\delta h_{0,q}[\rho]}{\delta\rho_{q'}}\delta\rho_{q'}\right]\phi_{q,i}(\boldsymbol{r}) \\
\left(-\hbar\omega + \epsilon_i - h_{0,q}\right)\delta\phi_{q,i}^{(+)}(\boldsymbol{r}) &= \left[v^{ext} + \sum_{q'}\frac{\delta h_{0,q}[\rho]}{\delta\rho_{q'}}\delta\rho_{q'}\right]^{\dagger}\phi_{q,i}(\boldsymbol{r})
\end{aligned}
$$

These two equations are the "Strurm-Liouville equation". The "Strurm-Liouville equation" takes the form $\boldsymbol{L}\Phi(\boldsymbol{r}) = -v(\boldsymbol{r})$, and the Green's function is defined as $\boldsymbol{L}G_{0,q}(\boldsymbol{r}\boldsymbol{r}') = -\delta(\boldsymbol{r}-\boldsymbol{r}')$. The solution can be given as $\Phi(\boldsymbol{r}) = \int d\boldsymbol{r}' G_{0,q}(\boldsymbol{r}\boldsymbol{r}')v(\boldsymbol{r}')$.

Here one can define Hartree-Fock Green's function as

$$
\left(\epsilon - h_{0,q}\right)G_{0,q}(\boldsymbol{r}\boldsymbol{r}';\epsilon) = -\delta(\boldsymbol{r}-\boldsymbol{r}')
$$

Note that the Lehman representation of the Green's function, with use of the orthogonality of the wave functions $\sum_i \phi_{q,i}(\boldsymbol{r})\phi_i^*(\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}')$, can be expressed as

$$
G_{0,q}(\boldsymbol{r}\boldsymbol{r}';\epsilon) = -\sum_{i\in all}\frac{\phi_{q,i}(\boldsymbol{r})\phi_{q,i}^*(\boldsymbol{r}')}{\epsilon - \epsilon_i}
$$

Therefore the solutions of above two equations can be given as

$$
\begin{aligned}
\delta\phi^{(-)}_{q,i}(\boldsymbol{r}) &= \int d\boldsymbol{r}' G_{0,q}(\boldsymbol{r}\boldsymbol{r}';\hbar\omega+\epsilon_i)\left[v^{ext}+\sum_{q'}\frac{\delta h_{0,q}[\rho]}{\delta\rho_{q'}}\delta\rho_{q'}\right]\phi_{q,i}(\boldsymbol{r}') \\
&= \int d\boldsymbol{r}' \sum_{j\in all}\frac{\phi_{q,j}(\boldsymbol{r})\phi^*_{q,j}(\boldsymbol{r}')}{\epsilon_j-\epsilon_i-\hbar\omega}\left[v^{ext}+\sum_{q'}\frac{\delta h_{0,q}[\rho]}{\delta\rho_{q'}}\delta\rho_{q'}\right]\phi_{q,i}(\boldsymbol{r}') \\
\delta\phi^{(+)}_{q,i}(\boldsymbol{r}) &= \int d\boldsymbol{r}' G_{0,q}(\boldsymbol{r}\boldsymbol{r}';-\hbar\omega+\epsilon_i)\left[v^{ext}+\sum_{q'}\frac{\delta h_{0,q}[\rho]}{\delta\rho_{q'}}\delta\rho_{q'}\right]^{\dagger}\phi_{q,i}(\boldsymbol{r}') \\
&= \int d\boldsymbol{r}' \sum_{j\in all}\frac{\phi_{q,j}(\boldsymbol{r})\phi^*_{q,j}(\boldsymbol{r}')}{\epsilon_j-\epsilon_i+\hbar\omega}\left[v^{ext}+\sum_{q'}\frac{\delta h_{0,q}[\rho]}{\delta\rho_{q'}}\delta\rho_{q'}\right]^{\dagger}\phi_{q,i}(\boldsymbol{r}')
\end{aligned}
$$

With use of the Skyrme interaction,

$$
\begin{aligned}
&\frac{\delta h_{0,q}[\rho]}{\delta\rho_{q'}}\delta\rho_{q'}\phi_{q,i}(\boldsymbol{r}) = \int d\boldsymbol{r}'\frac{\delta h_{0,q}[\rho]\phi_{q,i}(\boldsymbol{r})}{\delta\rho_{q'}(\boldsymbol{r}')}\delta\rho_{q'}(\boldsymbol{r}') \\
&= -\left(B_3+\delta_{qq'}B_4\right)\delta\rho_{q'}(\boldsymbol{r})\Delta\phi_{q,i}(\boldsymbol{r}) + \left(B_3+\delta_{qq'}B_4\right)\left[2i\delta\boldsymbol{j}_{q'}(\boldsymbol{r})-\nabla\delta\rho_{q'}(\boldsymbol{r})\right]\cdot\nabla\phi_{q,i}(\boldsymbol{r}) \\
&\quad+\Big[2B_1+\delta_{qq'}2B_2+(\alpha+2)(\alpha+1)B_7\rho^{\alpha}(\boldsymbol{r}) \\
&\qquad +\alpha(\alpha-1)B_8\rho^{\alpha-2}(\boldsymbol{r})\sum_{q''}\rho^2_{q''}(\boldsymbol{r})+2\alpha B_8\rho^{\alpha-1}(\boldsymbol{r})\left(\rho_{q'}(\boldsymbol{r})+\rho_q(\boldsymbol{r})\right)+2B_8\rho^{\alpha}(\boldsymbol{r})\delta_{qq'}\Big]\delta\rho_{q'}(\boldsymbol{r})\phi_{q,i}(\boldsymbol{r}) \\
&\quad+\left[\left(B_3+\delta_{qq'}B_4\right)\left(\delta\tau_{q'}(\boldsymbol{r})+i\nabla\cdot\delta\boldsymbol{j}_{q'}(\boldsymbol{r})\right)+\left(2B_5+\delta_{qq'}2B_6\right)\Delta\delta\rho_{q'}(\boldsymbol{r})\right]\phi_{q,i}(\boldsymbol{r}) \\
&= 2b_{qq'}\delta\rho_{q'}(\boldsymbol{r})\Delta\phi_{q,i}(\boldsymbol{r}) - 2b_{qq'}\left[2i\delta\boldsymbol{j}_{q'}(\boldsymbol{r})-\nabla\delta\rho_{q'}(\boldsymbol{r})\right]\cdot\nabla\phi_{q,i}(\boldsymbol{r}) + a_{qq'}(\boldsymbol{r})\delta\rho_{q'}(\boldsymbol{r})\phi_{q,i}(\boldsymbol{r}) \\
&\quad -2b_{qq'}\left(\delta\tau_{q'}(\boldsymbol{r})+i\nabla\cdot\delta\boldsymbol{j}_{q'}(\boldsymbol{r})\right)\phi_{q,i}(\boldsymbol{r}) + \left(2b_{qq'}-c_{qq'}\right)\Delta\delta\rho_{q'}(\boldsymbol{r})\phi_{q,i}(\boldsymbol{r})
\end{aligned}
$$

Therefore

$$
\begin{aligned}
\int d\boldsymbol{r}'\phi^*_{q,j}(\boldsymbol{r}')\frac{\delta h_{0,q}[\rho]}{\delta\rho_{q'}}\delta\rho_{q'}\phi_{q,i}(\boldsymbol{r}') &= \int d\boldsymbol{r}'\phi^*_{q,j}(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}')a_{qq'}(\boldsymbol{r}')\delta\rho_{q'}(\boldsymbol{r}') \\
&+\int d\boldsymbol{r}'\phi^*_{q,j}(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}')b_{qq'}\Delta_{+}\delta\rho_{q'}(\boldsymbol{r}') \\
&+\int d\boldsymbol{r}'\phi^*_{q,j}(\boldsymbol{r}')\left(\overleftarrow{\nabla}-\overrightarrow{\nabla}\right)\phi_{q,i}(\boldsymbol{r}')b_{qq'}\cdot 2i\delta\boldsymbol{j}_{q'}(\boldsymbol{r}') \\
&+\int d\boldsymbol{r}'\phi^*_{q,j}(\boldsymbol{r}')\left(\overleftarrow{\nabla}+\overrightarrow{\nabla}\right)\phi_{q,i}(\boldsymbol{r}')c_{qq'}\nabla\delta\rho_{q'}(\boldsymbol{r}') \\
&+\int d\boldsymbol{r}'\phi^*_{q,j}(\boldsymbol{r}')\left(\overleftarrow{\Delta}+\overrightarrow{\Delta}\right)\phi_{q,i}(\boldsymbol{r}')b_{qq'}\delta\rho_{q'}(\boldsymbol{r}')
\end{aligned}
$$

And also

$$
\begin{aligned}
\int d\boldsymbol{r}'\phi^*_{q,j}(\boldsymbol{r}')\left[\frac{\delta h_{0,q}[\rho]}{\delta\rho_{q'}}\delta\rho_{q'}\right]^\dagger \phi_{q,i}(\boldsymbol{r}') &= \left[\int d\boldsymbol{r}'\phi^*_{q,i}(\boldsymbol{r}')\frac{\delta h_{0,q}[\rho]}{\delta\rho_{q'}}\delta\rho_{q'}\phi_{q,j}(\boldsymbol{r}')\right]^* \\
&= \Bigg[\int d\boldsymbol{r}'\phi^*_{q,i}(\boldsymbol{r}')\phi_{q,j}(\boldsymbol{r}')a_{qq'}(\boldsymbol{r}')\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \int d\boldsymbol{r}'\phi^*_{q,i}(\boldsymbol{r}')\phi_{q,j}(\boldsymbol{r}')b_{qq'}\Delta_+\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \int d\boldsymbol{r}'\phi^*_{q,i}(\boldsymbol{r}')\left(\overleftarrow{\nabla}-\overrightarrow{\nabla}\right)\phi_{q,j}(\boldsymbol{r}')b_{qq'}\cdot 2i\delta\boldsymbol{j}_{q'}(\boldsymbol{r}') \\
&\quad + \int d\boldsymbol{r}'\phi^*_{q,i}(\boldsymbol{r}')\left(\overleftarrow{\nabla}+\overrightarrow{\nabla}\right)\phi_{q,j}(\boldsymbol{r}')c_{qq'}\nabla\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \int d\boldsymbol{r}'\phi^*_{q,i}(\boldsymbol{r}')\left(\overleftarrow{\Delta}+\overrightarrow{\Delta}\right)\phi_{q,j}(\boldsymbol{r}')b_{qq'}\delta\rho_{q'}(\boldsymbol{r}')\Bigg]^* \\
&= \int d\boldsymbol{r}'\phi^*_{q,j}(\boldsymbol{r}')\frac{\delta h_{0,q}[\rho]}{\delta\rho_{q'}}\delta\rho_{q'}\phi_{q,i}(\boldsymbol{r}')
\end{aligned}
$$

Then one can get

$$
\begin{aligned}
\delta\phi^{(-)}_{q,i}(\boldsymbol{r}) &= \int d\boldsymbol{r}'\sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}')v^{ext} \\
&\quad + \int d\boldsymbol{r}'\sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}')\sum_{q'}a_{qq'}(\boldsymbol{r}')\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \int d\boldsymbol{r}'\sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}')\sum_{q'}b_{qq'}\Delta_+\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \int d\boldsymbol{r}'\sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\left(\overleftarrow{\Delta}'+\overrightarrow{\Delta}'\right)\phi_{q,i}(\boldsymbol{r}')\sum_{q'}b_{qq'}\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \int d\boldsymbol{r}'\sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\left(\overleftarrow{\nabla}'+\overrightarrow{\nabla}'\right)\phi_{q,i}(\boldsymbol{r}')\sum_{q'}c_{qq'}\nabla_+\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \int d\boldsymbol{r}'\sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\left(\overleftarrow{\nabla}'-\overrightarrow{\nabla}'\right)\phi_{q,i}(\boldsymbol{r}')\sum_{q'}b_{qq'}2i\delta\boldsymbol{j}_{q'}(\boldsymbol{r}')
\end{aligned}
$$

$$
\begin{aligned}
\delta\phi^{(+)}_{q,i}(\boldsymbol{r}) &= \int d\boldsymbol{r}'\sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}')v^{ext} \\
&\quad + \int d\boldsymbol{r}'\sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}')\sum_{q'}a_{qq'}(\boldsymbol{r}')\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \int d\boldsymbol{r}'\sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}')\sum_{q'}b_{qq'}\Delta_+\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \int d\boldsymbol{r}'\sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\left(\overleftarrow{\Delta}'+\overrightarrow{\Delta}'\right)\phi_{q,i}(\boldsymbol{r}')\sum_{q'}b_{qq'}\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \int d\boldsymbol{r}'\sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\left(\overleftarrow{\nabla}'+\overrightarrow{\nabla}'\right)\phi_{q,i}(\boldsymbol{r}')\sum_{q'}c_{qq'}\nabla_+\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \int d\boldsymbol{r}'\sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\left(\overleftarrow{\nabla}'-\overrightarrow{\nabla}'\right)\phi_{q,i}(\boldsymbol{r}')\sum_{q'}b_{qq'}2i\delta\boldsymbol{j}_{q'}(\boldsymbol{r}')
\end{aligned}
$$

Here we define the transition density

$$
\begin{aligned}
\rho_q(\boldsymbol{r},t) &= \sum_i \phi^*_{q,i}(\boldsymbol{r},t)\phi_{q,i}(\boldsymbol{r},t) \\
&= \sum_i \phi^*_{q,i}(\boldsymbol{r})\phi_{q,i}(\boldsymbol{r}) \qquad \to \rho_q(\boldsymbol{r}) \\
&\quad + e^{i\omega t}\sum_i \left\{\phi^*_{q,i}(\boldsymbol{r})\delta\phi^{(-)}_{q,i}(\boldsymbol{r}) + \phi_{q,i}(\boldsymbol{r})\delta\phi^{(+)*}_{q,i}(\boldsymbol{r})\right\} \qquad \to e^{-i\omega t}\delta\rho_q(\boldsymbol{r}) \\
&\quad + h.c. \qquad \to e^{i\omega t}\delta\rho^*_q(\boldsymbol{r})
\end{aligned}
$$

Linear responce equation

$$
\begin{aligned}
\delta\rho_q(\boldsymbol{r}) &= \sum_i \left\{\phi^*_{q,i}(\boldsymbol{r})\delta\phi^{(-)}_{q,i}(\boldsymbol{r}) + \phi_{q,i}(\boldsymbol{r})\delta\phi^{(+)*}_{q,i}(\boldsymbol{r})\right\} \\
&= \int d\boldsymbol{r}' \sum_{i\in bound}\Bigg[\phi^*_{q,i}(\boldsymbol{r})\Bigg\{\sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}')v^{ext} \\
&\quad + \sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}')\sum_{q'}a_{qq'}(\boldsymbol{r}')\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}')\sum_{q'}b_{qq'}\Delta_+\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\left(\overleftarrow{\Delta}'+\overrightarrow{\Delta}'\right)\phi_{q,i}(\boldsymbol{r}')\sum_{q'}b_{qq'}\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\left(\overleftarrow{\nabla}'+\overrightarrow{\nabla}'\right)\phi_{q,i}(\boldsymbol{r}')\sum_{q'}c_{qq'}\nabla_+\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \sum_{j\in all}\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\left(\overleftarrow{\nabla}'-\overrightarrow{\nabla}'\right)\phi_{q,i}(\boldsymbol{r}')\sum_{q'}b_{qq'}2i\delta\boldsymbol{j}_{q'}(\boldsymbol{r}')\Bigg\} \\
&\quad + \phi_{q,i}(\boldsymbol{r})\Bigg\{\sum_{j\in all}\phi^*_{q,i}(\boldsymbol{r}')\phi_{q,j}(\boldsymbol{r}')\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega}\phi^*_{q,j}(\boldsymbol{r})v^{ext} \\
&\quad + \sum_{j\in all}\phi^*_{q,i}(\boldsymbol{r}')\phi_{q,j}(\boldsymbol{r}')\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega}\phi^*_{q,j}(\boldsymbol{r})\sum_{q'}a_{qq'}(\boldsymbol{r}')\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \sum_{j\in all}\phi^*_{q,i}(\boldsymbol{r}')\phi_{q,j}(\boldsymbol{r}')\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega}\phi^*_{q,j}(\boldsymbol{r})\sum_{q'}b_{qq'}\Delta_+\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \sum_{j\in all}\phi^*_{q,i}(\boldsymbol{r}')\left(\overleftarrow{\Delta}'+\overrightarrow{\Delta}'\right)\phi_{q,j}(\boldsymbol{r}')\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega}\phi^*_{q,j}(\boldsymbol{r})\sum_{q'}b_{qq'}\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \sum_{j\in all}\phi^*_{q,i}(\boldsymbol{r}')\left(\overleftarrow{\nabla}'+\overrightarrow{\nabla}'\right)\phi_{q,j}(\boldsymbol{r}')\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega}\phi^*_{q,j}(\boldsymbol{r})\sum_{q'}c_{qq'}\nabla_+\delta\rho_{q'}(\boldsymbol{r}') \\
&\quad + \sum_{j\in all}\phi^*_{q,i}(\boldsymbol{r}')\left(\overleftarrow{\nabla}'-\overrightarrow{\nabla}'\right)\phi_{q,j}(\boldsymbol{r}')\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega}\phi^*_{q,j}(\boldsymbol{r})\sum_{q'}b_{qq'}2i\delta\boldsymbol{j}_{q'}(\boldsymbol{r}')\Bigg\}^*\Bigg]
\end{aligned}
$$

Here one define the responce function

$$
\begin{aligned}
&\sum_{i\in bound}\sum_{j\in all}\Bigg\{\phi^*_{q,i}(\boldsymbol{r})\hat{O}_\alpha(\boldsymbol{r})\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega}\phi^*_{q,j}(\boldsymbol{r}')\hat{O}_\beta(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}') \\
&\qquad\qquad +\phi^*_{q,j}(\boldsymbol{r})\hat{O}_\alpha(\boldsymbol{r})\phi_{q,i}(\boldsymbol{r})\phi^*_{q,i}(\boldsymbol{r}')\hat{O}_\beta(\boldsymbol{r}')\phi_{q,j}(\boldsymbol{r}')\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega}\Bigg\} \\
&=\sum_{i\in bound}\Bigg\{\phi^*_{q,i}(\boldsymbol{r})\hat{O}_\alpha(\boldsymbol{r})G_{0,q}(\boldsymbol{r}\boldsymbol{r}';\hbar\omega+\epsilon_i)\hat{O}_\beta(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}')+\phi^*_{q,i}(\boldsymbol{r}')\hat{O}_\beta(\boldsymbol{r}')G_{0,q}(\boldsymbol{r}'\boldsymbol{r};-\hbar\omega+\epsilon_i)\hat{O}_\alpha(\boldsymbol{r})\phi_{q,i}(\boldsymbol{r})\Bigg\} \\
&\equiv R^{\alpha\beta}_{0,q}(\boldsymbol{r}\boldsymbol{r}';\omega)
\end{aligned}
$$

where

$$\hat{O}_\alpha(\boldsymbol{r}),\hat{O}_\beta(\boldsymbol{r})\in\Big\{1,\overleftarrow{\nabla}+\overrightarrow{\nabla},\overleftarrow{\nabla}-\overrightarrow{\nabla},\overleftarrow{\Delta}+\overrightarrow{\Delta}\Big\}$$

The linear responce equation is

$$\delta\rho_{\alpha,q}(\boldsymbol{r}) = \sum_\beta\int d\boldsymbol{r}'\left[R^{\alpha\beta}_{0,q}(\boldsymbol{r}\boldsymbol{r}';\omega)\sum_{q'}v^{ph,qq'}_\beta(\boldsymbol{r}')\delta\rho_{\beta,q'}(\boldsymbol{r}')+R^{\alpha 1}_{0,q}(\boldsymbol{r}\boldsymbol{r}';\omega)v^{ext}_q(\boldsymbol{r}')\right]$$

3.5.1 Strength function and energy-weighted sum rule

The linear responce equation becomes

$$
\begin{aligned}
\delta\rho_{\alpha,q}(\boldsymbol{r}) &= \int d\boldsymbol{r}'R^{\alpha 1}_{0,q}(\boldsymbol{r}\boldsymbol{r}';\omega)v^{ext}_q(\boldsymbol{r}') \\
&\quad+\sum_\beta\int d\boldsymbol{r}'\left[R^{\alpha\beta}_{0,q}(\boldsymbol{r}\boldsymbol{r}';\omega)\sum_{q'}v^{ph,qq'}_\beta(\boldsymbol{r}')\delta\rho_{\beta,q'}(\boldsymbol{r}')\right] \\
&= \int d\boldsymbol{r}'R^{\alpha 1}_{0,q}(\boldsymbol{r}\boldsymbol{r}';\omega)v^{ext}_q(\boldsymbol{r}') \\
&\quad+\sum_\beta\int d\boldsymbol{r}'\int d\boldsymbol{r}''\left[R^{\alpha\beta}_{0,q}(\boldsymbol{r}\boldsymbol{r}';\omega)\sum_{q'}v^{ph,qq'}_\beta(\boldsymbol{r}')R^{\beta 1}_{0,q'}(\boldsymbol{r}'\boldsymbol{r}'';\omega)v^{ext}_{q'}(\boldsymbol{r}'')\right] \\
&\quad+\sum_{\beta,\beta'\cdots}\int d\boldsymbol{r}'\int d\boldsymbol{r}''\cdots\left[R^{\alpha\beta}_{0,q}(\boldsymbol{r}\boldsymbol{r}';\omega)\sum_{q'}v^{ph,qq'}_\beta(\boldsymbol{r}')R^{\beta\beta'}_{0,q'}(\boldsymbol{r}'\boldsymbol{r}'';\omega)\sum_{q''}v^{ph,q'q''}_{\beta'}(\boldsymbol{r}'')\cdots\right]
\end{aligned}
$$

The strength function and its energy-weighted sum are defined as

$$
\begin{aligned}
S_q(\hbar\omega) &= -\frac{1}{\pi}\mathrm{Im}\int d\boldsymbol{r}v^{ext,*}_q(\boldsymbol{r})\delta\rho_{1,q}(\boldsymbol{r}) \\
&= -\frac{1}{\pi}\mathrm{Im}\int d\boldsymbol{r}v^{ext,*}_q(\boldsymbol{r})\Bigg[\int d\boldsymbol{r}'R^{11}_{0,q}(\boldsymbol{r}\boldsymbol{r}';\omega)v^{ext}_q(\boldsymbol{r}') \\
&\quad+\sum_\beta\int d\boldsymbol{r}'\int d\boldsymbol{r}''\left\{R^{1\beta}_{0,q}(\boldsymbol{r}\boldsymbol{r}';\omega)\sum_{q'}v^{ph,qq'}_\beta(\boldsymbol{r}')R^{\beta 1}_{0,q'}(\boldsymbol{r}'\boldsymbol{r}'';\omega)v^{ext}_{q'}(\boldsymbol{r}'')\right\}+\cdots\Bigg] \\
&= -\frac{1}{\pi}\mathrm{Im}\int d\boldsymbol{r}\int d\boldsymbol{r}'v^{ext,*}_q(\boldsymbol{r})R^{11}_{0,q}(\boldsymbol{r}\boldsymbol{r}';\omega)v^{ext}_q(\boldsymbol{r}') \\
&\quad-\sum_\beta\sum_{q'}\frac{1}{\pi}\mathrm{Im}\int d\boldsymbol{r}\int d\boldsymbol{r}'\int d\boldsymbol{r}''v^{ext,*}_q(\boldsymbol{r})R^{1\beta}_{0,q}(\boldsymbol{r}\boldsymbol{r}';\omega)v^{ph,qq'}_\beta(\boldsymbol{r}')R^{\beta 1}_{0,q'}(\boldsymbol{r}'\boldsymbol{r}'';\omega)v^{ext}_{q'}(\boldsymbol{r}'') \\
&= -\frac{1}{\pi}\mathrm{Im}\langle v^{ext,*}_qR^{11}_{0,q}(\omega)v^{ext}_q\rangle-\frac{1}{\pi}\sum_\beta\sum_{q'}\mathrm{Im}\langle v^{ext,*}_qR^{1\beta}_{0,q}(;\omega)v^{ph,qq'}_\beta R^{\beta 1}_{0,q'}(;\omega)v^{ext}_{q'}\rangle
\end{aligned}
$$

The contribution for the energy-weighted sum of the first term is

$$
\begin{aligned}
&\frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\omega\langle v_q^{ext,*}R_{0,q}^{11}(\omega)v_q^{ext}\rangle \\
&= \frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\int d\boldsymbol{r}\int d\boldsymbol{r}'\omega\sum_{i\in bound}\sum_{j\in all}\Bigg\{\phi_{q,i}^*(\boldsymbol{r})v_q^{ext,*}(\boldsymbol{r})\phi_{q,j}(\boldsymbol{r})\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega-i\epsilon}\phi_{q,j}^*(\boldsymbol{r}')v_q^{ext}(\boldsymbol{r}')\phi_{q,i}(\boldsymbol{r}') \\
&\qquad\qquad +\phi_{q,j}^*(\boldsymbol{r})v_q^{ext,*}(\boldsymbol{r})\phi_{q,i}(\boldsymbol{r})\phi_{q,i}^*(\boldsymbol{r}')v_q^{ext}(\boldsymbol{r}')\phi_{q,j}(\boldsymbol{r}')\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega-i\epsilon}\Bigg\} \\
&= \frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\omega\sum_{i\in bound}\sum_{j\in all}|\langle i|v_q^{ext}|j\rangle|^2\Bigg\{\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega-i\epsilon}+\frac{1}{\epsilon_j-\epsilon_i+\hbar\omega-i\epsilon}\Bigg\} \\
&= \frac{1}{\pi}\mathrm{Im}\int_{-\infty}^\infty d\omega\omega\sum_{i\in bound}\sum_{j\in all}|\langle i|v_q^{ext}|j\rangle|^2\Bigg\{\frac{1}{\epsilon_j-\epsilon_i-\hbar\omega-i\epsilon}\Bigg\} \\
&= \frac{1}{\pi}\mathrm{Im}\int_{-\infty}^\infty d\omega\omega\sum_{i\in bound}\sum_{j\in all}|\langle i|v_q^{ext}|j\rangle|^2\hbar\Bigg\{\mathrm{P}\frac{1}{\frac{\epsilon_j-\epsilon_i}{\hbar}-\omega}+i\pi\delta(\frac{\epsilon_j-\epsilon_i}{\hbar}-\omega)\Bigg\} \\
&= \sum_{i\in bound}\sum_{j\in all}(\epsilon_j-\epsilon_i)|\langle i|v_q^{ext}|j\rangle|^2=\sum_{p,h}(\epsilon_p-\epsilon_h)|\langle h|v_q^{ext}|p\rangle|^2
\end{aligned}
$$

On the other hand, the double commutator relation of Hartree-Fock hamiltonian $\hat{h}_0$ and the external field $\hat{f}$ becomes

$$
\begin{aligned}
\langle 0|\left[\hat{f},\left[\hat{h}_0,\hat{f}\right]\right]|0\rangle &= \sum_{p,h}\langle 0|\left[\hat{f},|ph\rangle\langle ph|\left[\hat{h}_0,\hat{f}\right]\right]|0\rangle \\
&= \sum_{p,h}\langle 0|\hat{f}|ph\rangle\langle ph|\left[\hat{h}_0,\hat{f}\right]|0\rangle=-\sum_{p,h}(\epsilon_p-\epsilon_h)|\langle h|\hat{f}|p\rangle|^2
\end{aligned}
$$

where

$$
\begin{aligned}
&\hat{h}_0|ph\rangle=(\epsilon_p-\epsilon_h)|ph\rangle \qquad \hat{h}_0|0\rangle=0 \qquad \langle 0|\hat{f}|ph\rangle=f_{hp}=\langle h|\hat{f}|p\rangle \\
&\hat{h}_0=\sum_i\epsilon_i:c_i^\dagger c_i:=\sum_p\epsilon_p a_p^\dagger a_p-\sum_h\epsilon_h b_h^\dagger b_h \qquad \hat{f}=\sum_{i,j}f_{ij}c_i^\dagger c_j
\end{aligned}
$$

And also, one can get from the coordinate space representatin Hartree-Fock hamiltonian,

$$
\langle 0|\left[\hat{f},\left[\hat{h}_0,\hat{f}\right]\right]|0\rangle=\langle\frac{\hbar^2}{m^*}[\nabla f]^2\rangle
$$

Therefore, the energy-weightes sum of the first term can be obtained as

$$
\frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\omega\langle v_q^{ext,*}R_{0,q}^{11}(\omega)v_q^{ext}\rangle=-\langle 0|\left[\hat{V}_q^{ext},\left[\hat{h}_0,\hat{V}_q^{ext}\right]\right]|0\rangle=-\langle\frac{\hbar^2}{m_q^*}[\nabla v_q^{ext}]^2\rangle
$$

The contribution of the second term is

$$
\begin{aligned}
&\frac{1}{\pi}\sum_{\beta}\sum_{q'}\mathrm{Im}\int_0^\infty d\omega\omega\langle v_q^{ext,*}R_{0,q}^{1\beta}(;\omega)v_\beta^{ph,qq'}R_{0,q'}^{\beta 1}(;\omega)v_{q'}^{ext}\rangle \\
&=\sum_{\beta}\sum_{q'}\frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\omega\int d\boldsymbol{r}\int d\boldsymbol{r}'\int d\boldsymbol{r}'' v_q^{ext,*}(\boldsymbol{r})R_{0,q}^{1\beta}(\boldsymbol{r}\boldsymbol{r}';\omega)v_\beta^{ph,qq'}(\boldsymbol{r}')R_{0,q'}^{\beta 1}(\boldsymbol{r}'\boldsymbol{r}'';\omega)v_{q'}^{ext}(\boldsymbol{r}'') \\
&=\sum_{q'}\frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\omega\int d\boldsymbol{r}\int d\boldsymbol{r}' a_{qq'}(\boldsymbol{r}')\int d\boldsymbol{r}'' v_q^{ext,*}(\boldsymbol{r})R_{0,q}^{11}(\boldsymbol{r}\boldsymbol{r}';\omega)R_{0,q'}^{11}(\boldsymbol{r}'\boldsymbol{r}'';\omega)v_{q'}^{ext}(\boldsymbol{r}'') \\
&\quad+\sum_{q'}\frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\omega\int d\boldsymbol{r}\int d\boldsymbol{r}' b_{qq'}\int d\boldsymbol{r}'' v_q^{ext,*}(\boldsymbol{r})R_{0,q}^{11}(\boldsymbol{r}\boldsymbol{r}';\omega)R_{0,q'}^{11}(\boldsymbol{r}'\boldsymbol{r}'';\omega)v_{q'}^{ext}(\boldsymbol{r}'') \\
&\quad+\sum_{q'}\frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\omega\int d\boldsymbol{r}\int d\boldsymbol{r}' b_{qq'}\int d\boldsymbol{r}'' v_q^{ext,*}(\boldsymbol{r})R_{0,q}^{1\Delta}(\boldsymbol{r}\boldsymbol{r}';\omega)R_{0,q'}^{\Delta 1}(\boldsymbol{r}'\boldsymbol{r}'';\omega)v_{q'}^{ext}(\boldsymbol{r}'') \\
&\quad+\sum_{q'}\frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\omega\int d\boldsymbol{r}\int d\boldsymbol{r}' c_{qq'}\int d\boldsymbol{r}'' v_q^{ext,*}(\boldsymbol{r})R_{0,q}^{1\nabla_+}(\boldsymbol{r}\boldsymbol{r}';\omega)R_{0,q'}^{\nabla_+ 1}(\boldsymbol{r}'\boldsymbol{r}'';\omega)v_{q'}^{ext}(\boldsymbol{r}'') \\
&\quad+\sum_{q'}\frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\omega\int d\boldsymbol{r}\int d\boldsymbol{r}' b_{qq'}\int d\boldsymbol{r}'' v_q^{ext,*}(\boldsymbol{r})R_{0,q}^{1\nabla_-}(\boldsymbol{r}\boldsymbol{r}';\omega)R_{0,q'}^{\nabla_- 1}(\boldsymbol{r}'\boldsymbol{r}'';\omega)v_{q'}^{ext}(\boldsymbol{r}'')
\end{aligned}
$$

where

$$
\begin{aligned}
\int d\boldsymbol{r} v_q^{ext,*}(\boldsymbol{r}) R_{0,q}^{1\beta}(\boldsymbol{r}\boldsymbol{r}';\omega) &= \int d\boldsymbol{r} \sum_{p,h} \Bigg\{ \phi_{q,h}^*(\boldsymbol{r}) v_q^{ext,*}(\boldsymbol{r}) \phi_{q,p}(\boldsymbol{r}) \frac{1}{\epsilon_p - \epsilon_h - \hbar\omega - i\epsilon} \phi_{q,p}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q,h}(\boldsymbol{r}') \\
&\quad + \phi_{q,p}^*(\boldsymbol{r}) v_q^{ext,*}(\boldsymbol{r}) \phi_{q,h}(\boldsymbol{r}) \phi_{q,h}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q,p}(\boldsymbol{r}') \frac{1}{\epsilon_p - \epsilon_h + \hbar\omega - i\epsilon} \Bigg\} \\
&= \sum_{p,h} \Bigg\{ \frac{1}{\epsilon_p - \epsilon_h - \hbar\omega - i\epsilon} \langle p | v_q^{ext} | h \rangle^* \phi_{q,p}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q,h}(\boldsymbol{r}') \\
&\quad + \frac{1}{\epsilon_p - \epsilon_h + \hbar\omega - i\epsilon} \langle h | v_q^{ext} | p \rangle^* \phi_{q,h}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q,p}(\boldsymbol{r}') \Bigg\}
\end{aligned}
$$

$$
\begin{aligned}
\int d\boldsymbol{r}'' R_{0,q}^{\beta 1}(\boldsymbol{r}'\boldsymbol{r}'';\omega) v_q^{ext}(\boldsymbol{r}'') &= \int d\boldsymbol{r}'' \sum_{p',h'} \Bigg\{ \phi_{q,h'}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q,p'}(\boldsymbol{r}') \frac{1}{\epsilon_{p'} - \epsilon_{h'} - \hbar\omega - i\epsilon} \phi_{q,p'}^*(\boldsymbol{r}'') v_q^{ext}(\boldsymbol{r}') \phi_{q,h'}(\boldsymbol{r}'') \\
&\quad + \phi_{q,p'}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q,h'}(\boldsymbol{r}') \phi_{q,h'}^*(\boldsymbol{r}'') v_q^{ext}(\boldsymbol{r}'') \phi_{q,p'}(\boldsymbol{r}'') \frac{1}{\epsilon_{p'} - \epsilon_{h'} + \hbar\omega - i\epsilon} \Bigg\} \\
&= \sum_{p',h'} \Bigg\{ \phi_{q,h'}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q,p'}(\boldsymbol{r}') \langle p' | v_q^{ext} | h' \rangle \frac{1}{\epsilon_{p'} - \epsilon_{h'} - \hbar\omega - i\epsilon} \\
&\quad + \phi_{q,p'}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q,h'}(\boldsymbol{r}') \langle h' | v_q^{ext} | p' \rangle \frac{1}{\epsilon_{p'} - \epsilon_{h'} + \hbar\omega - i\epsilon} \Bigg\} \\
\langle ij | V_{qq'}^{ph} | kl \rangle &\equiv \sum_\beta \int d\boldsymbol{r}' \left[\phi_{q,i}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q,j}(\boldsymbol{r}') \right] v_\beta^{ph,qq'}(\boldsymbol{r}') \left[\phi_{q',k}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q',l}(\boldsymbol{r}') \right] \\
&= \langle kl | V_{qq'}^{ph} | ij \rangle
\end{aligned}
$$

$$
\begin{aligned}
\langle ij | V_{qq'}^{ph} | kl \rangle^* &\equiv \left[\sum_\beta \int d\boldsymbol{r}' \left[\phi_{q,i}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q,j}(\boldsymbol{r}') \right] v_\beta^{ph,qq'}(\boldsymbol{r}') \left[\phi_{q',k}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q',l}(\boldsymbol{r}') \right] \right]^* \\
&= \sum_\beta \int d\boldsymbol{r}' \left[\phi_{q',l}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q',k}(\boldsymbol{r}') \right] v_\beta^{ph,qq'}(\boldsymbol{r}') \left[\phi_{q,j}^*(\boldsymbol{r}') \hat{O}_\beta(\boldsymbol{r}') \phi_{q,i}(\boldsymbol{r}') \right] \\
&= \langle lk | V_{qq'}^{ph} | ji \rangle = \langle ji | V_{qq'}^{ph} | lk \rangle
\end{aligned}
$$

$$
\begin{aligned}
&\sum_{q'}\frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\omega\sum_\beta\int d\boldsymbol{r'}\left[\int d\boldsymbol{r}v_q^{ext,*}(\boldsymbol{r})R_{0,q}^{1\beta}(\boldsymbol{rr'};\omega)v_\beta^{ph,qq'}(\boldsymbol{r'})\int d\boldsymbol{r''}R_{0,q'}^{\beta 1}(\boldsymbol{r'r''};\omega)v_{q'}^{ext}(\boldsymbol{r''})\right]\\
&=\sum_{q'}\frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\omega\sum_{p,p'}\sum_{h,h'}\frac{1}{\epsilon_p-\epsilon_h-\hbar\omega-i\epsilon}\langle p|v_q^{ext}|h\rangle^*\\
&\qquad\times\left\{\langle ph|V_{qq'}^{ph}|h'p'\rangle\langle p'|v_{q'}^{ext}|h'\rangle\frac{1}{\epsilon_{p'}-\epsilon_{h'}-\hbar\omega-i\epsilon}+\langle ph|V_{qq'}^{ph}|p'h'\rangle\langle h'|v_{q'}^{ext}|p'\rangle\frac{1}{\epsilon_{p'}-\epsilon_{h'}+\hbar\omega-i\epsilon}\right\}\\
&+\sum_{q'}\frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\omega\sum_{p,p'}\sum_{h,h'}\frac{1}{\epsilon_p-\epsilon_h+\hbar\omega-i\epsilon}\langle h|v_q^{ext}|p\rangle^*\\
&\qquad\times\left\{\langle hp|V_{qq'}^{ph}|h'p'\rangle\langle p'|v_{q'}^{ext}|h'\rangle\frac{1}{\epsilon_{p'}-\epsilon_{h'}-\hbar\omega-i\epsilon}+\langle hp|V_{qq'}^{ph}|p'h'\rangle\langle h'|v_{q'}^{ext}|p'\rangle\frac{1}{\epsilon_{p'}-\epsilon_{h'}+\hbar\omega-i\epsilon}\right\}\\
&=\sum_{q'}\frac{1}{\pi}\mathrm{Im}\int_0^\infty d\omega\omega\sum_{p,p'}\sum_{h,h'}\frac{1}{\epsilon_p-\epsilon_h-\hbar\omega-i\epsilon}\\
&\times\left\{\langle h|v_q^{ext,*}|p\rangle\langle ph|V_{qq'}^{ph}|h'p'\rangle\langle p'|v_{q'}^{ext}|h'\rangle\frac{1}{\epsilon_{p'}-\epsilon_{h'}-\hbar\omega-i\epsilon}\right.\\
&\qquad\qquad\left.+\langle h|v_q^{ext,*}|p\rangle\langle ph|V_{qq'}^{ph}|p'h'\rangle\langle h'|v_{q'}^{ext}|p'\rangle\frac{1}{\epsilon_{p'}-\epsilon_{h'}+\hbar\omega-i\epsilon}\right\}\\
&+\sum_{q'}\frac{1}{\pi}\mathrm{Im}\int_{-\infty}^0 d\omega\omega\sum_{p,p'}\sum_{h,h'}\frac{1}{\epsilon_p-\epsilon_h-\hbar\omega-i\epsilon}\\
&\times\left\{\langle p|v_q^{ext,*}|h\rangle\langle hp|V_{qq'}^{ph}|h'p'\rangle\langle p'|v_{q'}^{ext}|h'\rangle\frac{1}{\epsilon_{p'}-\epsilon_{h'}+\hbar\omega-i\epsilon}\right.\\
&\qquad\qquad\left.+\langle p|v_q^{ext,*}|h\rangle\langle hp|V_{qq'}^{ph}|p'h'\rangle\langle h'|v_{q'}^{ext}|p'\rangle\frac{1}{\epsilon_{p'}-\epsilon_{h'}-\hbar\omega-i\epsilon}\right\}
\end{aligned}
$$

Appendix A

Isospin operator

If we consider only neutron and proton system, isospin operators have the properties as

$$\hat{\boldsymbol{t}}^2|q\rangle = \frac{1}{2}\left(\frac{1}{2}+1\right)|q\rangle \qquad \hat{t}_z|q\rangle = \pm\frac{1}{2}|q\rangle \begin{cases} + & (q=n: neutron) \\ - & (q=p: proton) \end{cases}$$

where $\hat{\boldsymbol{t}} = \frac{1}{2}\boldsymbol{\tau}$. τ is the Pauli's spin matrices.
So

$$[\tau_i, \tau_j] = 2i\epsilon_{ijk}\tau_k \qquad \left([\hat{t}_i, \hat{t}_j] = i\epsilon_{ijk}\hat{t}_k\right)$$

The isospin ladder operators can be defined as

$$\hat{t}_\pm = \hat{t}_x \pm i\hat{t}_y \qquad \begin{cases} \hat{t}_+|p\rangle = |n\rangle & \hat{t}_-|p\rangle = 0 \\ \hat{t}_-|n\rangle = |p\rangle & \hat{t}_+|n\rangle = 0 \end{cases}$$

A.1.2 2 particle system

$$\begin{aligned} \hat{\boldsymbol{t}}_1\cdot\hat{\boldsymbol{t}}_2 &= \hat{t}_{1x}\hat{t}_{2x} + \hat{t}_{1y}\hat{t}_{2y} + \hat{t}_{1z}\hat{t}_{2z} = \frac{1}{2}\left(\hat{t}_{1+}\hat{t}_{2-} + \hat{t}_{1-}\hat{t}_{2+}\right) + \hat{t}_{1z}\hat{t}_{2z} \\ \hat{\boldsymbol{\tau}}_1\cdot\hat{\boldsymbol{\tau}}_2 &= 2\left(\hat{t}_{1+}\hat{t}_{2-} + \hat{t}_{1-}\hat{t}_{2+} + 2\hat{t}_{1z}\hat{t}_{2z}\right) \end{aligned}$$

$$\begin{pmatrix} \langle nn|\tau_1\cdot\tau_2|nn\rangle & \langle nn|\tau_1\cdot\tau_2|np\rangle & \langle nn|\tau_1\cdot\tau_2|pn\rangle & \langle nn|\tau_1\cdot\tau_2|pp\rangle \\ \langle np|\tau_1\cdot\tau_2|nn\rangle & \langle np|\tau_1\cdot\tau_2|np\rangle & \langle np|\tau_1\cdot\tau_2|pn\rangle & \langle np|\tau_1\cdot\tau_2|pp\rangle \\ \langle pn|\tau_1\cdot\tau_2|nn\rangle & \langle pn|\tau_1\cdot\tau_2|np\rangle & \langle pn|\tau_1\cdot\tau_2|pn\rangle & \langle pn|\tau_1\cdot\tau_2|pp\rangle \\ \langle pp|\tau_1\cdot\tau_2|nn\rangle & \langle pp|\tau_1\cdot\tau_2|np\rangle & \langle pp|\tau_1\cdot\tau_2|pn\rangle & \langle pp|\tau_1\cdot\tau_2|pp\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\tau_1\cdot\tau_2 \rightarrow \langle qq'|\tau_1\cdot\tau_2|qq'\rangle = 2\delta_{qq'} - 1 = \begin{cases} (q=q'): & 1 \\ (q\neq q'): & -1 \end{cases}$$

$$\begin{aligned} \hat{\boldsymbol{T}} &= \hat{\boldsymbol{t}}_1 + \hat{\boldsymbol{t}}_2 \\ \hat{\boldsymbol{T}}^2 &= \left(\hat{\boldsymbol{t}}_1 + \hat{\boldsymbol{t}}_2\right)^2 = \hat{\boldsymbol{t}}_1^2 + \hat{\boldsymbol{t}}_2^2 + 2\hat{\boldsymbol{t}}_1\cdot\hat{\boldsymbol{t}}_2 = \frac{3}{2} + \frac{1}{2}\hat{\boldsymbol{\tau}}_1\cdot\hat{\boldsymbol{\tau}}_2 \quad\rightarrow\quad \hat{\boldsymbol{\tau}}_1\cdot\hat{\boldsymbol{\tau}}_2 = 2\hat{\boldsymbol{T}}^2 - 3 \end{aligned}$$

Here one defines $|TT_z\rangle\rangle$

$$\begin{aligned} \hat{\boldsymbol{T}}^2|TT_z\rangle\rangle &= T(T+1)|TT_z\rangle\rangle \\ \hat{T}_z|TT_z\rangle\rangle &= T_z|TT_z\rangle\rangle \end{aligned}$$

$$|1,1\rangle\rangle = |nn\rangle, \qquad |1,0\rangle\rangle = \frac{1}{\sqrt{2}}\left(|np\rangle + |pn\rangle\right), \qquad |1,-1\rangle\rangle = |pp\rangle, \qquad |0,0\rangle\rangle = \frac{1}{\sqrt{2}}\left(|np\rangle - |pn\rangle\right)$$

By using these kets, the matrix elements of $\tau_1 \cdot \tau_2$ become

$$\begin{pmatrix} \langle\langle 1+1|\tau_1\cdot\tau_2|1+1\rangle\rangle & \langle\langle 1+1|\tau_1\cdot\tau_2|1,0\rangle\rangle & \langle\langle 1+1|\tau_1\cdot\tau_2|1-1\rangle\rangle & \langle\langle 1+1|\tau_1\cdot\tau_2|0,0\rangle\rangle \\ \langle\langle 1,0|\tau_1\cdot\tau_2|1+1\rangle\rangle & \langle\langle 1,0|\tau_1\cdot\tau_2|1,0\rangle\rangle & \langle\langle 1,0|\tau_1\cdot\tau_2|1-1\rangle\rangle & \langle\langle 1,0|\tau_1\cdot\tau_2|0,0\rangle\rangle \\ \langle\langle 1-1|\tau_1\cdot\tau_2|1+1\rangle\rangle & \langle\langle 1-1|\tau_1\cdot\tau_2|1,0\rangle\rangle & \langle\langle 1-1|\tau_1\cdot\tau_2|1-1\rangle\rangle & \langle\langle 1-1|\tau_1\cdot\tau_2|0,0\rangle\rangle \\ \langle\langle 0,0|\tau_1\cdot\tau_2|1+1\rangle\rangle & \langle\langle 0,0|\tau_1\cdot\tau_2|1,0\rangle\rangle & \langle\langle 0,0|\tau_1\cdot\tau_2|1-1\rangle\rangle & \langle\langle 0,0|\tau_1\cdot\tau_2|0,0\rangle\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}$$

A.2 Exchange operator

The spin and isospin exchange operators are given by

$$P_\sigma(12) \equiv \frac{1}{2}\left(1 + \boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}\right) \qquad P_\tau(12) \equiv \frac{1}{2}\left(1 + \boldsymbol{\tau_1}\cdot\boldsymbol{\tau_2}\right)$$

because spin, isospin operators $\boldsymbol{\tau_1}\cdot\boldsymbol{\tau_2}$, $\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}$ can be expressed as

$$\hat{\boldsymbol{\sigma}}_1\cdot\hat{\boldsymbol{\sigma}}_2 = 2\left(\hat{s}_{1+}\hat{s}_{2-} + \hat{s}_{1-}\hat{s}_{2+} + 2\hat{s}_{1z}\hat{s}_{2z}\right), \qquad \hat{\boldsymbol{\tau}}_1\cdot\hat{\boldsymbol{\tau}}_2 = 2\left(\hat{t}_{1+}\hat{t}_{2-} + \hat{t}_{1-}\hat{t}_{2+} + 2\hat{t}_{1z}\hat{t}_{2z}\right)$$

then

$$P_\sigma(12)|\sigma_1\sigma_2\rangle = |\sigma_2\sigma_1\rangle \qquad P_\tau(12)|q_1q_2\rangle = |q_2q_1\rangle$$

Appendix B

The Density Functional Derivatives

The density functional derivatives can be defined as

$$\frac{\delta F[f(x)]}{\delta f(y)} = \lim_{\epsilon \to 0} \frac{F[f(x) + \epsilon\delta(x-y)] - F[f(x)]}{\epsilon}$$

Example(1)

$$\begin{aligned}
F[\rho(x)] &= \rho(x)^2 \\
\frac{\delta F[\rho(x)]}{\delta \rho(y)} &= \lim_{\epsilon \to 0} \frac{F[\rho(x) + \epsilon\delta(x-y)] - F[\rho(x)]}{\epsilon} \\
&= \lim_{\epsilon \to 0} \frac{(\rho(x) + \epsilon\delta(x-y))^2 - \rho(x)^2}{\epsilon} = \lim_{\epsilon \to 0} \frac{2\epsilon\delta(x-y)\rho(x) - \epsilon^2\delta^2(x-y)}{\epsilon} \\
&= 2\delta(x-y)\rho(x)
\end{aligned}$$

Example(2)

$$\begin{aligned}
F[\rho(x)] &= [\nabla_x \rho(x)]^2 \\
\frac{\delta F[\rho(x)]}{\delta \rho(y)} &= \lim_{\epsilon \to 0} \frac{F[\rho(x) + \epsilon\delta(x-y)] - F[\rho(x)]}{\epsilon} \\
&= \lim_{\epsilon \to 0} \frac{[\nabla_x \rho(x) + \epsilon\nabla_x\delta(x-y)]^2 - [\nabla_x\rho(x)]^2}{\epsilon} = \lim_{\epsilon \to 0} \frac{2\epsilon\nabla_x\rho(x)\nabla_x\delta(x-y) - \epsilon^2\left(\nabla_x\delta(x-y)\right)^2}{\epsilon} \\
&= 2\nabla_x\rho(x)\nabla_x\delta(x-y)
\end{aligned}$$

Then we can get the result

$$\int dy \frac{\delta F[\rho(x)]}{\delta\rho(y)}\delta\rho(y) = 2\nabla_x\rho(x)\nabla_x\delta\rho(x)$$

Functional derivative of the current density term

Next we will show the special example, we think the current density.
The current density can be defined as

$$j(x) \equiv \frac{1}{2i}\left(\nabla_x\rho(x,x')|_{x'=x} - \nabla_{x'}\rho(x,x')|_{x'=x}\right)$$

$$\int dy \frac{\delta j^2(x)}{\delta\rho(y)}\delta\rho(y) \quad = \quad \int dy 2j(x)\frac{\delta j(x)}{\delta\rho(y)}\delta\rho(y) = 2j(x)\int\int dydy'\delta(y-y')\frac{\delta j(x)}{\delta\rho(yy')}\delta\rho(yy')$$

Because the right hand side of above should be $2j(x)\delta j(x)$, then

$$\frac{\delta j(x)}{\delta\rho(yy')} = \frac{1}{2i}\left(\delta(x'-y')\nabla_x\delta(x-y)|_{x'=x} - \delta(x-y)\nabla_{x'}\delta(x'-y')|_{x'=x}\right)$$

$$\int\int dydy'\delta(y-y')\frac{\delta j(x)}{\delta\rho(yy')}\delta\rho(yy') = \frac{1}{2i}\left\{\nabla_x\left(\delta(x-x')\delta\rho(xx')\right)-\nabla_{x'}\left(\delta(x-x')\delta\rho(xx')\right)\right\}|_{x'=x}$$
$$= \frac{1}{2i}\left\{\nabla_x\delta\rho(xx')-\nabla_{x'}\delta\rho(xx')\right\}|_{x'=x}=\delta j(x)$$

Functional 2nd derivative of the current density term

$$\int\int dx_1dx_2f(x_1)\left[\int dy\frac{\delta^2 j^2(x)}{\delta\rho(x_1x_2)\delta\rho(y)}\delta\rho(y)\right]g(x_2)=\int\int dx_1dx_2\;2\left[f(x_1)\frac{\delta j(x)}{\delta\rho(x_1x_2)}g(x_2)\right]\delta j(x)$$
$$=\int\int dx_1dx_2\left[f(x_1)\frac{1}{i}\left(\delta(x'-x_2)\nabla_x\delta(x-x_1)|_{x'=x}-\delta(x-x_1)\nabla_{x'}\delta(x'-x_2)|_{x'=x}\right)g(x_2)\right]\delta j(x)$$
$$=\frac{1}{i}\left[f(x)\left(\overleftarrow{\nabla}-\overrightarrow{\nabla}\right)g(x)\right]\delta j(x)=-\frac{1}{2}\left[f(x)\left(\overleftarrow{\nabla}-\overrightarrow{\nabla}\right)g(x)\right]\nabla_-\delta\rho(x)$$

Example(3)

By following these rules for the calculation, we can also calculate the 2nd derivative of $\rho\tau$ in the energy functional with the Skyrme effective interaction.

$$\int\int dx_1dx_2f(x_1)\left[\int dy\frac{\delta^2\rho(x)\tau(x)}{\delta\rho(x_1x_2)\delta\rho(y)}\delta\rho(y)\right]g(x_2)=\int\int dx_1dx_2f(x_1)\frac{\delta}{\delta\rho(x_1x_2)}\left[\tau(x)\delta\rho(x)+\rho(x)\delta\tau(x)\right]g(x_2)$$
$$=\left[\int\int dx_1dx_2f(x_1)\frac{\delta\tau(x)}{\delta\rho(x_1x_2)}g(x_2)\right]\delta\rho(x)+f(x)g(x)\delta\tau(x)$$
$$=\frac{1}{2}\left[\Delta(f(x)g(x))-f(x)\left(\overleftarrow{\Delta}+\overrightarrow{\Delta}\right)g(x)\right]\delta\rho(x)+f(x)g(x)\frac{1}{2}\left(\Delta\delta\rho(x)-\Delta_+\delta\rho(x)\right)$$

If the last line is in the integration $\int dx$, the partial integration can be executed as

$$\int dx\left[\frac{1}{2}\left[\Delta(f(x)g(x))-f(x)\left(\overleftarrow{\Delta}+\overrightarrow{\Delta}\right)g(x)\right]\delta\rho(x)+f(x)g(x)\frac{1}{2}\left(\Delta\delta\rho(x)-\Delta_+\delta\rho(x)\right)\right]$$
$$=-\int dx\left[\frac{1}{2}\left[\nabla(f(x)g(x))\right]\nabla\delta\rho(x)+\frac{1}{2}\left[f(x)\left(\overleftarrow{\Delta}+\overrightarrow{\Delta}\right)g(x)\right]\delta\rho(x)+\frac{1}{2}\nabla\left(f(x)g(x)\right)\nabla\delta\rho(x)+\frac{1}{2}f(x)g(x)\Delta_+\delta\rho(x)\right]$$
$$=-\int dx\left[\left[f(x)\left(\overleftarrow{\nabla}+\overrightarrow{\nabla}\right)g(x)\right]\nabla\delta\rho(x)+\frac{1}{2}\left[f(x)\left(\overleftarrow{\Delta}+\overrightarrow{\Delta}\right)g(x)\right]\delta\rho(x)+\frac{1}{2}f(x)g(x)\Delta_+\delta\rho(x)\right]$$

Here we use

$$\tau(x)=\nabla_x\nabla_{x'}\rho(xx')|_{x'=x}=\frac{1}{2}\left(\Delta\rho(x)-\Delta_+\rho(x)\right)\qquad\text{where}\qquad\Delta_+\rho(x)=\Delta_x\rho(xx')|_{x'=x}+\Delta_{x'}\rho(xx')|_{x'=x}$$
$$\delta\tau(x)=\nabla_x\nabla_{x'}\delta\rho(xx')|_{x'=x}=\frac{1}{2}\left(\Delta\delta\rho(x)-\Delta_+\delta\rho(x)\right)\qquad\text{where}\qquad\Delta_+\delta\rho(x)=\Delta_x\delta\rho(xx')|_{x'=x}+\Delta_{x'}\delta\rho(xx')|_{x'=x}$$

Example(4)

$$\int\int dx_1dx_2f(x_1)\left[\int dy\frac{\delta^2\rho(x)\Delta\rho(x)}{\delta\rho(x_1x_2)\delta\rho(y)}\delta\rho(y)\right]g(x_2)=\int\int dx_1dx_2f(x_1)\frac{\delta}{\delta\rho(x_1x_2)}\left[\rho(x)\Delta\delta\rho(x)+\Delta\rho(x)\delta\rho(x)\right]g(x_2)$$
$$=f(x)g(x)\Delta\delta\rho(x)+\Delta\left(f(x)g(x)\right)\delta\rho(x)$$

If the last line is in the integration $\int dx$, the partial integration can be executed as

$$\int dx\left[f(x)g(x)\Delta\delta\rho(x)+\Delta\left(f(x)g(x)\right)\delta\rho(x)\right] = \int dx\left[-\nabla\left(f(x)g(x)\right)\nabla\delta\rho(x)-\nabla\left(f(x)g(x)\right)\cdot\nabla\delta\rho(x)\right]$$
$$= \int dx\left[-2f(x)\left(\overleftarrow{\nabla}+\overrightarrow{\nabla}\right)g(x)\cdot\nabla_+\delta\rho(x)\right]$$

Summary of examples

$$\int\int dx_1 dx_2 f(x_1)\left[\int dy \frac{\delta^2}{\delta\rho(x_1x_2)\delta\rho(y)}\left\{\int dx\rho(x)\tau(x)\right\}\delta\rho(y)\right]g(x_2)$$
$$=\int dx\left[-\left[f(x)\left(\overleftarrow{\nabla}+\overrightarrow{\nabla}\right)g(x)\right]\nabla\delta\rho(x)-\frac{1}{2}\left[f(x)\left(\overleftarrow{\Delta}+\overrightarrow{\Delta}\right)g(x)\right]\delta\rho(x)-\frac{1}{2}f(x)g(x)\Delta_+\delta\rho(x)\right]$$
$$\int\int dx_1 dx_2 f(x_1)\left[\int dy \frac{\delta^2}{\delta\rho(x_1x_2)\delta\rho(y)}\left\{\int dx\,\boldsymbol{j}^2(x)\right\}\delta\rho(y)\right]g(x_2)=-\frac{1}{2}\left[f(x)\left(\overleftarrow{\nabla}-\overrightarrow{\nabla}\right)g(x)\right]\cdot\nabla_-\delta\rho(x)$$
$$\int\int dx_1 dx_2 f(x_1)\left[\int dy \frac{\delta^2}{\delta\rho(x_1x_2)\delta\rho(y)}\left\{\int dx\rho(x)\Delta\rho(x)\right\}\delta\rho(y)\right]g(x_2)=\int dx\left[-2f(x)\left(\overleftarrow{\nabla}+\overrightarrow{\nabla}\right)g(x)\cdot\nabla_+\delta\rho(x)\right]$$

B.1 The energy functional with the Skyrme interaction

Skyrme effective interaction is given by

$$
\begin{aligned}
v(\boldsymbol{r}_1,\boldsymbol{r}_2) &= t_0(1+x_0P_\sigma)\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)+\frac{t_3}{6}(1+x_3P_\sigma)\rho^\alpha\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\\
&\quad+\frac{t_1}{2}(1+x_1P_\sigma)\left(\overleftarrow{k}^2+\overrightarrow{k}^2\right)\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)+t_2(1+x_2P_\sigma)\overleftarrow{\boldsymbol{k}}\cdot\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\overrightarrow{\boldsymbol{k}}\\
&\quad+iW_0\boldsymbol{\sigma}\cdot\overleftarrow{\boldsymbol{k}}\times\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\overrightarrow{\boldsymbol{k}}
\end{aligned}
$$

where $\overrightarrow{\boldsymbol{k}}=\frac{1}{2i}(\overrightarrow{\nabla}_1-\overrightarrow{\nabla}_2)$ is the relative momentum operator acting on the right, and $\overleftarrow{\boldsymbol{k}}=\frac{1}{2i}(\overleftarrow{\nabla}_1-\overleftarrow{\nabla}_2)$ is its adjoint action on the left.

The 2nd quantized Hamiltonian using 2-body interaction is given by

$$
\begin{aligned}
\hat{\mathrm{H}} &= \sum_{\sigma\tau}\int d\boldsymbol{r}\psi^\dagger(\boldsymbol{r}\sigma\tau)\frac{-\hbar^2}{2m}\nabla^2\psi(\boldsymbol{r}\sigma\tau)\\
&\quad+\frac{1}{4}\sum_{\sigma\sigma'}\sum_{\tau\tau'}\int\int d\boldsymbol{r}d\boldsymbol{r'}\psi^\dagger(\boldsymbol{r}\sigma\tau)\psi^\dagger(\boldsymbol{r'}\sigma'\tau')\tilde{v}(\boldsymbol{r},\boldsymbol{r'})\psi(\boldsymbol{r'}\sigma'\tau')\psi(\boldsymbol{r}\sigma\tau) \qquad \text{(B.1)}
\end{aligned}
$$

and its expectation value in the ground state is given by

$$
\begin{aligned}
\langle H_0\rangle &= \sum_{\sigma_1\sigma_2}\sum_{q_1q_2}\int\int d\boldsymbol{r}_1d\boldsymbol{r}_2T(1,2)\rho(2,1)\\
&\quad+\frac{1}{2}\sum_{\sigma_1\sim\sigma_4}\sum_{q_1\sim q_4}\int\overset{\cdots}{}\int d\boldsymbol{r}_1...d\boldsymbol{r}_4\langle 12|v_{12}(1-P)|34\rangle\rho(3,1)\rho(4,2)\\
&\quad+\frac{1}{2}\sum_{\sigma_1\sim\sigma_4}\sum_{q_1\sim q_4}\int\overset{\cdots}{}\int d\boldsymbol{r}_1...d\boldsymbol{r}_4\langle 12|v_{pair}(1-P)|34\rangle 2\sigma_2\sigma_4\tilde{\rho}^*(1,\bar{2})\tilde{\rho}(3,\bar{4})\\
&= \sum_{i=1}^{8}\langle H\rangle_i+\widetilde{\langle H\rangle}
\end{aligned}
$$

$$
\begin{aligned}
\langle H\rangle_1 &= \int d\boldsymbol{r}[\frac{\hbar^2}{2m}\tau(\boldsymbol{r})+B_1\rho^2(\boldsymbol{r})+B_2\sum_q\rho_q^2(\boldsymbol{r})]\\
\langle H\rangle_2 &= \int d\boldsymbol{r}B_3[\rho(\boldsymbol{r})\tau(\boldsymbol{r})-\boldsymbol{j}^2(\boldsymbol{r})]\\
\langle H\rangle_3 &= \int d\boldsymbol{r}B_4\sum_q[\rho_q(\boldsymbol{r})\tau_q(\boldsymbol{r})-\boldsymbol{j_q}^2(\boldsymbol{r})]\\
\langle H\rangle_4 &= \int d\boldsymbol{r}B_5\rho(\boldsymbol{r})\Delta\rho(\boldsymbol{r})\\
\langle H\rangle_5 &= \int d\boldsymbol{r}B_6\sum_q\rho_q(\boldsymbol{r})\Delta\rho_q(\boldsymbol{r})\\
\langle H\rangle_6 &= \int d\boldsymbol{r}(B_7\rho^{\alpha+2}(\boldsymbol{r})+B_8\rho^\alpha(\boldsymbol{r})\sum_q\rho_q^2(\boldsymbol{r}))\\
\langle H\rangle_7 &= \int d\boldsymbol{r}B_9\{(\rho(\boldsymbol{r})\nabla\cdot\boldsymbol{J}(\boldsymbol{r})+\boldsymbol{j}(\boldsymbol{r})\cdot\nabla\times\boldsymbol{\rho}(\boldsymbol{r}))\\
&\quad+\sum_q(\rho_q(\boldsymbol{r})\nabla\cdot\boldsymbol{J}_q(\boldsymbol{r})+\boldsymbol{j}_q(\boldsymbol{r})\cdot\nabla\times\boldsymbol{\rho}_q(\boldsymbol{r}))\}\\
\langle H\rangle_8 &= \int d\boldsymbol{r}[B_{10}\boldsymbol{\rho}^2(\boldsymbol{r})+B_{11}\sum_q\boldsymbol{\rho}_q^2(\boldsymbol{r})\\
&\quad+B_{12}\rho^\alpha(\boldsymbol{r})\boldsymbol{\rho}^2(\boldsymbol{r})+B_{13}\rho^\alpha(\boldsymbol{r})\sum_q\boldsymbol{\rho}_q^2(\boldsymbol{r})]
\end{aligned}
$$

$$
\widetilde{\langle H\rangle} = \frac{1}{4}V_0\left(1-\frac{\rho(r)}{\rho_0}\right)\int d\boldsymbol{r}\sum_q|\tilde{\rho}_q(\boldsymbol{r})|^2
$$

$$
\begin{aligned}
B_1 &= \frac{1}{2}t_0(1+\frac{1}{2}x_0), \qquad B_2=-\frac{1}{2}t_0(x_0+\frac{1}{2})\\
B_3 &= \frac{1}{4}\{t_1(1+\frac{1}{2}x_1)+t_2(1+\frac{1}{2}x_2)\}\\
B_4 &= -\frac{1}{4}\{t_1(x_1+\frac{1}{2})-t_2(x_2+\frac{1}{2})\}\\
B_5 &= -\frac{1}{16}\{3t_1(1+\frac{1}{2}x_1)-t_2(1+\frac{1}{2}x_2)\}\\
B_6 &= \frac{1}{16}\{3t_1(x_1+\frac{1}{2})+t_2(x_2+\frac{1}{2})\}\\
B_7 &= \frac{1}{12}t_3(1+\frac{1}{2}x_3), \qquad B_8=-\frac{1}{12}t_3(x_3+\frac{1}{2})\\
B_9 &= -\frac{1}{2}W, \qquad B_{10}=\frac{1}{4}t_0x_0, \qquad B_{11}=-\frac{1}{4}t_0,\\
B_{12} &= \frac{1}{24}t_3x_3, \qquad B_{13}=-\frac{1}{24}t_3
\end{aligned}
$$

$$
\begin{aligned}
\nabla\cdot\boldsymbol{J}(\boldsymbol{r}) &= -i\sum_{ijk}\epsilon_{ijk}\nabla_i\nabla'_j\rho_k(\boldsymbol{r},\boldsymbol{r'})\big|_{\boldsymbol{r'}=\boldsymbol{r}}\\
\tau(\boldsymbol{r}) &= \nabla\cdot\nabla'\rho(\boldsymbol{r},\boldsymbol{r'})\big|_{\boldsymbol{r'}=\boldsymbol{r}}\\
\boldsymbol{j}(\boldsymbol{r}) &= \frac{1}{2i}\left(\nabla\rho(\boldsymbol{r},\boldsymbol{r'})-\nabla'\rho(\boldsymbol{r},\boldsymbol{r'})\right)\big|_{\boldsymbol{r'}=\boldsymbol{r}}
\end{aligned}
$$

B.1.1 2nd derivative of the energy functional with the Skyrme interaction

$$\int d\boldsymbol{r}_1 f_q(\boldsymbol{r}_1)\left[\sum_{q'}\int d\boldsymbol{r}_2 \frac{\delta^2\langle H\rangle}{\delta\rho_q(\boldsymbol{r}_1)\delta\rho_{q'}(\boldsymbol{r}_2)}\delta\rho_{q'}(\boldsymbol{r}_2)\right] g_q(\boldsymbol{r}_1)$$

$$\int d\boldsymbol{r}_1 f_q(\boldsymbol{r}_1)\left[\sum_{q'}\int d\boldsymbol{r}_2 \frac{\delta^2\langle H\rangle_1}{\delta\rho_q(\boldsymbol{r}_1)\delta\rho_{q'}(\boldsymbol{r}_2)}\delta\rho_{q'}(\boldsymbol{r}_2)\right] g_q(\boldsymbol{r}_1) = \int d\boldsymbol{r}\left[f_q(\boldsymbol{r})g_q(\boldsymbol{r})\sum_{q'} 2\left\{B_1+\delta_{qq'}B_2\right\}\delta\rho_{q'}(\boldsymbol{r})\right]$$

$$\begin{aligned}
&\int d\boldsymbol{r}_1 f_q(\boldsymbol{r}_1)\left[\sum_{q'}\int d\boldsymbol{r}_2 \frac{\delta^2\langle H\rangle_2}{\delta\rho_q(\boldsymbol{r}_1)\delta\rho_{q'}(\boldsymbol{r}_2)}\delta\rho_{q'}(\boldsymbol{r}_2)\right] g_q(\boldsymbol{r}_1)\\
&\quad = \int d\boldsymbol{r}\Big[f_q(\boldsymbol{r})g_q(\boldsymbol{r})\sum_{q'}\left(-\frac{1}{2}B_3\right)\Delta_+\delta\rho_{q'}(\boldsymbol{r}) + f_q(\boldsymbol{r})\left(\overleftarrow{\Delta}+\overrightarrow{\Delta}\right)g_q(\boldsymbol{r})\sum_{q'}\left(-\frac{1}{2}B_3\right)\delta\rho_{q'}(\boldsymbol{r})\\
&\qquad + f_q(\boldsymbol{r})\left(\overleftarrow{\nabla}+\overrightarrow{\nabla}\right)g_q(\boldsymbol{r})\sum_{q'}(-B_3)\nabla_+\delta\rho_{q'}(\boldsymbol{r}) + f_q(\boldsymbol{r})\left(\overleftarrow{\nabla}-\overrightarrow{\nabla}\right)g_q(\boldsymbol{r})\sum_{q'}\left(-\frac{1}{2}B_3\right)\nabla_-\delta\rho_{q'}(\boldsymbol{r})\Big]
\end{aligned}$$

$$\begin{aligned}
&\int d\boldsymbol{r}_1 f_q(\boldsymbol{r}_1)\left[\sum_{q'}\int d\boldsymbol{r}_2 \frac{\delta^2\langle H\rangle_3}{\delta\rho_q(\boldsymbol{r}_1)\delta\rho_{q'}(\boldsymbol{r}_2)}\delta\rho_{q'}(\boldsymbol{r}_2)\right] g_q(\boldsymbol{r}_1)\\
&\quad = \int d\boldsymbol{r}\Big[f_q(\boldsymbol{r})g_q(\boldsymbol{r})\sum_{q'}\left(-\frac{1}{2}\delta_{qq'}B_4\right)\Delta_+\delta\rho_{q'}(\boldsymbol{r}) + f_q(\boldsymbol{r})\left(\overleftarrow{\Delta}+\overrightarrow{\Delta}\right)g_q(\boldsymbol{r})\sum_{q'}\left(-\frac{1}{2}\delta_{qq'}B_4\right)\delta\rho_{q'}(\boldsymbol{r})\\
&\qquad + f_q(\boldsymbol{r})\left(\overleftarrow{\nabla}+\overrightarrow{\nabla}\right)g_q(\boldsymbol{r})\sum_{q'}(-\delta_{qq'}B_4)\nabla_+\delta\rho_{q'}(\boldsymbol{r}) + f_q(\boldsymbol{r})\left(\overleftarrow{\nabla}-\overrightarrow{\nabla}\right)g_q(\boldsymbol{r})\sum_{q'}\left(-\frac{1}{2}\delta_{qq'}B_4\right)\nabla_-\delta\rho_{q'}(\boldsymbol{r})\Big]
\end{aligned}$$

$$\begin{aligned}
&\int d\boldsymbol{r}_1 f_q(\boldsymbol{r}_1)\left[\sum_{q'}\int d\boldsymbol{r}_2 \frac{\delta^2\langle H\rangle_4}{\delta\rho_q(\boldsymbol{r}_1)\delta\rho_{q'}(\boldsymbol{r}_2)}\delta\rho_{q'}(\boldsymbol{r}_2)\right] g_q(\boldsymbol{r}_1)\\
&\quad = \int d\boldsymbol{r}\left[f_q(\boldsymbol{r})\left(\overleftarrow{\nabla}+\overrightarrow{\nabla}\right)g_q(\boldsymbol{r})\sum_{q'}\left(-2B_5\right)\nabla_+\delta\rho_{q'}(\boldsymbol{r})\right]
\end{aligned}$$

$$\begin{aligned}
&\int d\boldsymbol{r}_1 f_q(\boldsymbol{r}_1)\left[\sum_{q'}\int d\boldsymbol{r}_2 \frac{\delta^2\langle H\rangle_5}{\delta\rho_q(\boldsymbol{r}_1)\delta\rho_{q'}(\boldsymbol{r}_2)}\delta\rho_{q'}(\boldsymbol{r}_2)\right] g_q(\boldsymbol{r}_1)\\
&\quad = \int d\boldsymbol{r}\left[f_q(\boldsymbol{r})\left(\overleftarrow{\nabla}+\overrightarrow{\nabla}\right)g_q(\boldsymbol{r})\sum_{q'}\left(-2\delta_{qq'}B_6\right)\nabla_+\delta\rho_{q'}(\boldsymbol{r})\right]
\end{aligned}$$

$$\begin{aligned}
&\int d\boldsymbol{r}_1 f_q(\boldsymbol{r}_1)\left[\sum_{q'}\int d\boldsymbol{r}_2 \frac{\delta^2\langle H\rangle_6}{\delta\rho_q(\boldsymbol{r}_1)\delta\rho_{q'}(\boldsymbol{r}_2)}\delta\rho_{q'}(\boldsymbol{r}_2)\right] g_q(\boldsymbol{r}_1)\\
&\quad = \int d\boldsymbol{r}\Bigg[f_q(\boldsymbol{r})g_q(\boldsymbol{r})\sum_{q'}\Bigg\{B_7(\alpha+2)(\alpha+1)\rho^{\alpha}(\boldsymbol{r}) + B_8\alpha(\alpha-1)\rho^{\alpha-2}(\boldsymbol{r})\left(\sum_{q''}\rho_{q''}^2(\boldsymbol{r})\right)\\
&\qquad + 2B_8\alpha\rho^{\alpha-1}(\boldsymbol{r})\left(\rho_q(\boldsymbol{r})+\rho_{q'}(\boldsymbol{r})\right) + 2\delta_{qq'}B_8\rho^{\alpha}\Bigg\}\delta\rho_{q'}(\boldsymbol{r})\Bigg]
\end{aligned}$$

Then summarized the calculation as,

$$\int d\boldsymbol{r}_1 f_q(\boldsymbol{r}_1)\left[\sum_{q'}\int d\boldsymbol{r}_2\frac{\delta^2\langle H\rangle}{\delta\rho_q(\boldsymbol{r}_1)\delta\rho_{q'}(\boldsymbol{r}_2)}\delta\rho_{q'}(\boldsymbol{r}_2)\right]g_q(\boldsymbol{r}_1)$$
$$=\int d\boldsymbol{r}\left[f_q(\boldsymbol{r})g_q(\boldsymbol{r})\sum_{q'}a_{qq'}(\boldsymbol{r})\delta\rho_{q'}(\boldsymbol{r})+f_q(\boldsymbol{r})\left(\overleftarrow{\Delta}+\overrightarrow{\Delta}\right)g_q(\boldsymbol{r})\sum_{q'}b_{qq'}\delta\rho_{q'}(\boldsymbol{r})+f_q(\boldsymbol{r})g_q(\boldsymbol{r})\sum_{q'}b_{qq'}\Delta_+\delta\rho_{q'}(\boldsymbol{r})\right.$$
$$\left.+f_q(\boldsymbol{r})\left(\overleftarrow{\nabla}+\overrightarrow{\nabla}\right)g_q(\boldsymbol{r})\sum_{q'}c_{qq'}\nabla_+\delta\rho_{q'}(\boldsymbol{r})+f_q(\boldsymbol{r})\left(\overleftarrow{\nabla}-\overrightarrow{\nabla}\right)g_q(\boldsymbol{r})\sum_{q'}b_{qq'}\nabla_-\delta\rho_{q'}(\boldsymbol{r})\right.$$

where

$$\begin{aligned}
a_{qq'}(\rho(\boldsymbol{r})) &= 2B_1+2\delta_{qq'}B_2+B_7(\alpha+2)(\alpha+1)\rho^\alpha(\boldsymbol{r})\\
&\qquad +B_8\alpha(\alpha-1)\rho^{\alpha-2}(\boldsymbol{r})\left(\sum_{q''}\rho^2_{q''}(\boldsymbol{r})\right)+2B_8\alpha\rho^{\alpha-1}(\boldsymbol{r})\left(\rho_q(\boldsymbol{r})+\rho_{q'}(\boldsymbol{r})\right)+2\delta_{qq'}B_8\rho^\alpha\\
&= \begin{cases} (q=q') & \frac{1}{2}t_0(1-x_0)+(\alpha+2)(\alpha+1)\frac{1}{12}t_3(1+\frac{1}{2}x_3)\rho^\alpha \\ & \quad -\frac{1}{12}t_3(x_3+\frac{1}{2})\left(\alpha(\alpha-1)\rho^{\alpha-2}\sum_{q''}\rho^2_{q''}+4\alpha\rho^{\alpha-1}\rho_q+2\rho^\alpha\right) \\ (q\neq q') & t_0(1+\frac{1}{2}x_0)+(\alpha+2)(\alpha+1)\frac{1}{12}t_3(1+\frac{1}{2}x_3)\rho^\alpha \\ & \quad -\frac{1}{12}t_3(x_3+\frac{1}{2})\left(\alpha(\alpha-1)\rho^{\alpha-2}\sum_{q''}\rho^2_{q''}+2\alpha\rho^\alpha\right) \end{cases}\\
b_{qq'} &= -\frac{1}{2}\left(B_3+\delta_{qq'}B_4\right)\\
&= \begin{cases} (q=q') & -\frac{1}{16}\left(t_1(1-x_1)+3t_2(1+x_2)\right) \\ (q\neq q') & -\frac{1}{8}\{t_1(1+\frac{1}{2}x_1)+t_2(1+\frac{1}{2}x_2)\} \end{cases}\\
c_{qq'} &= -\left(B_3+2B_5\right)-\delta_{qq'}\left(B_4+2B_6\right)\\
&= \begin{cases} (q=q') & -\frac{1}{16}\left(t_1(x_1-1)+9t_2(x_2+1)\right) \\ (q\neq q') & \frac{1}{8}\{t_1(1+\frac{1}{2}x_1)-3t_2(1+\frac{1}{2}x_2)\} \end{cases}
\end{aligned}$$

In *Sagawa*'s paper, he defined

$$\begin{array}{ll} \rho=\rho_n+\rho_p, & \rho_t=\rho_n-\rho_p \\ \rho^2=\rho_n^2+\rho_p^2+2\rho_n\rho_p, & \rho_t^2=\rho_n^2+\rho_p^2-2\rho_n\rho_p \end{array}$$
$$\rightarrow\qquad \sum_q\rho_q^2=\frac{1}{2}\left(\rho^2+\rho_t^2\right)$$

and using

$$\tau_1\!\cdot\!\tau_2\rightarrow\langle qq'|\tau_1\!\cdot\!\tau_2|qq'\rangle=2\delta_{qq'}-1=\begin{cases}(q=q'): & 1\\ (q\neq q'): & -1\end{cases}$$

Then the residual interaction a, b and c are expressed as

$$\begin{aligned}
a_{qq'} &= \frac{3}{4}t_0+\frac{1}{12}t_3(1+\frac{1}{2}x_3)(\alpha+2)(\alpha+1)\rho^\alpha(\boldsymbol{r})\\
&\quad -\frac{1}{12}t_3(x_3+\frac{1}{2})\rho^\alpha-\frac{1}{48}t_3(2x_3+1)\alpha(\alpha-1)\rho^{\alpha-2}(\boldsymbol{r})\left(\rho^2+\rho_t^2\right)\\
&\quad -\frac{1}{6}t_3(x_3+\frac{1}{2})\alpha\rho^{\alpha-1}(\boldsymbol{r})\left(\frac{1}{2}\left(1+\tau_1\!\cdot\!\tau_2\right)(2\rho_q-\rho)+\rho\right)-\tau_1\!\cdot\!\tau_2\left(\frac{1}{4}t_0(2x_0+1)+\frac{1}{24}t_3(2x_3+1)\rho^\alpha\right)\\
&= \frac{3}{4}t_0+\frac{3}{48}t_3(\alpha+2)(\alpha+1)\rho^\alpha-\frac{1}{48}t_3(2x_3+1)\alpha(\alpha-1)\rho^{\alpha-2}\rho_t^2-\tau_1\!\cdot\!\tau_2\left(\frac{1}{4}t_0(2x_0+1)+\frac{1}{24}t_3(2x_3+1)\rho^\alpha\right)\\
&\quad -\frac{1}{12}t_3(2x_3+1)\alpha\rho^{\alpha-1}(\boldsymbol{r})\frac{1}{2}\left(1+\tau_1\!\cdot\!\tau_2\right)(2\rho_q-\rho)\\
b_{qq'} &= -\frac{1}{32}\left(3t_1+t_2(5+4x_2)\right)+\tau_1\!\cdot\!\tau_2\frac{1}{32}\left(t_1(2x_1+1)-t_2(2x_2+1)\right)\\
c_{qq'} &= \frac{1}{32}\left(3t_1-t_2(15+12x_2)\right)-\tau_1\!\cdot\!\tau_2\frac{1}{32}\left(t_1(1+2x_1)+3t_2(1+2x_2)\right)
\end{aligned}$$

where one used a below relation too,

$$\begin{aligned}
\rho_q + \rho_{q'} &= (\delta_{qq'} + (1-\delta_{qq'}))(\rho_q + \rho_{q'}) \\
&= \delta_{qq'}(\rho_q + \rho_{q'}) + (1-\delta_{qq'})(\rho_q + \rho_{q'}) \\
&= 2\delta_{qq'}\rho_q + (1-\delta_{qq'})\rho \\
&= \delta_{qq'}(2\rho_q - \rho) + \rho = \frac{1}{2}(1+\tau_1\cdot\tau_2)(2\rho_q - \rho) + \rho
\end{aligned}$$

B.2 Sum rule with the Skyrme interaction

Hartree-Fock mean field Hamiltonian can be defined as

$$\hat{h}_{HF} \equiv \iint d\boldsymbol{r}_1 d\boldsymbol{r}_2 \psi^\dagger(\boldsymbol{r}_1)\frac{\delta\langle H\rangle}{\delta\rho(\boldsymbol{r}_2\boldsymbol{r}_1)}\psi(\boldsymbol{r}_2) = \iint d\boldsymbol{r}_1 d\boldsymbol{r}_2 \frac{\delta\langle H\rangle}{\delta\rho(\boldsymbol{r}_2\boldsymbol{r}_1)}\psi^\dagger(\boldsymbol{r}_1)\psi(\boldsymbol{r}_2)$$

Residual interaction can be also defined as

$$\begin{aligned}
\hat{h}_V &\equiv \frac{1}{2}\int\!\!\int\!\!\cdots\!\!\int d\boldsymbol{r}_1\cdots d\boldsymbol{r}_4 \psi^\dagger(\boldsymbol{r}_1)\psi^\dagger(\boldsymbol{r}_2)\frac{\delta^2\langle H\rangle}{\delta\rho(\boldsymbol{r}_4\boldsymbol{r}_1)\delta\rho(\boldsymbol{r}_3\boldsymbol{r}_2)}\psi(\boldsymbol{r}_3)\psi(\boldsymbol{r}_4) \\
&= \frac{1}{2}\int\!\!\int\!\!\cdots\!\!\int d\boldsymbol{r}_1\cdots d\boldsymbol{r}_4 \psi^\dagger(\boldsymbol{r}_1)\psi(\boldsymbol{r}_4)\frac{\delta^2\langle H\rangle}{\delta\rho(\boldsymbol{r}_4\boldsymbol{r}_1)\delta\rho(\boldsymbol{r}_3\boldsymbol{r}_2)}\psi^\dagger(\boldsymbol{r}_2)\psi(\boldsymbol{r}_3)
\end{aligned}$$

Here I note that field operators take “Normal order”. So the expectation value for the HF ground state is zero. That is

$$\langle 0|\hat{h}_{HF} + \hat{h}_V|0\rangle = 0$$

B.2.1 Hartree-Fock Mean field Hamiltonian with Skyrme interaction

If one uses the Skyrme interaction keeping with the velocity dependent terms, the Hartree-Fock mean field Hamiltonian is given by

$$\begin{aligned}
\hat{h}_{HF} &= \int d\boldsymbol{r}\left[\left\{\frac{\hbar^2}{2m} + B_3\rho(\boldsymbol{r})\right\}\hat{\tau}(\boldsymbol{r}) + B_4\sum_q \rho_q(\boldsymbol{r})\hat{\tau}_q(\boldsymbol{r})\right] \\
&\quad - \int d\boldsymbol{r}\left[2B_5\nabla\rho(\boldsymbol{r})\nabla\hat{\rho}(\boldsymbol{r}) + \sum_q 2B_6\nabla\rho_q(\boldsymbol{r})\nabla\hat{\rho}_q(\boldsymbol{r})\right] \\
&\quad + \int d\boldsymbol{r}\left[\{2B_1\rho(\boldsymbol{r}) + B_3\tau(\boldsymbol{r})\}\hat{\rho}(\boldsymbol{r}) + \sum_q\{2B_2\rho_q(\boldsymbol{r}) + B_4\tau_q(\boldsymbol{r})\}\hat{\rho}_q(\boldsymbol{r})\right]
\end{aligned}$$

where $\hat{\rho}_{(q)}, \hat{\tau}_{(q)}$, and $\nabla\hat{\rho}_{(q)}$ are defined as

$$\begin{cases}
\hat{\rho}(\boldsymbol{r}) &= \sum_q \psi_q^\dagger(\boldsymbol{r})\psi_q(\boldsymbol{r}) = \sum_q \hat{\rho}_q(\boldsymbol{r}) \\
\hat{\tau}(\boldsymbol{r}) &= \sum_q \nabla\psi_q^\dagger(\boldsymbol{r})\cdot\nabla\psi_q(\boldsymbol{r}) = \sum_q \hat{\tau}_q(\boldsymbol{r}) \\
\nabla\hat{\rho}(\boldsymbol{r}) &= \sum_q \psi_q^\dagger(\boldsymbol{r})\left(\overleftarrow{\nabla} + \overrightarrow{\nabla}\right)\psi_q(\boldsymbol{r}) = \sum_q \nabla\hat{\rho}_q(\boldsymbol{r})
\end{cases}$$

Important double commutator relations

$$\begin{aligned}
\langle 0|[\hat{\rho}(\boldsymbol{r}''), [\hat{\tau}(\boldsymbol{r}), \hat{\rho}(\boldsymbol{r}')]]|0\rangle &= 2\left[\rho(\boldsymbol{r}', \boldsymbol{r}'')\nabla\delta(\boldsymbol{r}-\boldsymbol{r}')\cdot\nabla\delta(\boldsymbol{r}-\boldsymbol{r}'') - \nabla\rho(\boldsymbol{r}, \boldsymbol{r}'')\cdot\delta(\boldsymbol{r}'-\boldsymbol{r}'')\nabla\delta(\boldsymbol{r}-\boldsymbol{r}')\right] \\
\langle 0|[\hat{\rho}(\boldsymbol{r}''), [\nabla\hat{\rho}(\boldsymbol{r}), \hat{\rho}(\boldsymbol{r}')]]|0\rangle &= 0 = \langle 0|[\hat{\rho}(\boldsymbol{r}''), [\hat{\rho}(\boldsymbol{r}), \hat{\rho}(\boldsymbol{r}')]]|0\rangle
\end{aligned}$$

By using these relations, one can the double commutator relations

$$\begin{aligned}\langle 0|\left[\hat{F},\left[\hat{h}_{HF},\hat{F}\right]\right]|0\rangle &= \int d\boldsymbol{r}\sum_q\left[\frac{\hbar^2}{m}+2B_3\rho(\boldsymbol{r})+2B_4\rho_q(\boldsymbol{r})\right]\rho_q(\boldsymbol{r})\left(\nabla f(r)\right)^2 \\ &= \int d\boldsymbol{r}\sum_q\left[\frac{\hbar^2}{m_q^*(\boldsymbol{r})}\right]\rho_q(\boldsymbol{r})\left(\nabla f(r)\right)^2\end{aligned}$$

where an 1-body isoscalar-type operator $\hat{F}$ is given by

$$\hat{F}=\int d\boldsymbol{r} f(\boldsymbol{r})\sum_q\psi_q^\dagger(\boldsymbol{r})\psi_q(\boldsymbol{r})=\int d\boldsymbol{r} f(\boldsymbol{r})\hat{\rho}(\boldsymbol{r})$$

(On the other hand, isovector-type operator is
$$\hat{F}=\int d\boldsymbol{r}\sum_q f_q(\boldsymbol{r})\hat{\rho}_q(\boldsymbol{r})$$
)

Note that, by replacing $f(\boldsymbol{r})$ with $f_q(\boldsymbol{r})$, one can get the double commutator relation for the isovector-type operator.

B.2.2 Residual interaction Hamiltonian with Skyrme interaction

If one keeps same terms with the previous subsection, the resdual hamiltonian is given by

$$\begin{aligned}\hat{h}_V &= \int d\boldsymbol{r}\left[B_3\left\{\hat{\rho}(\boldsymbol{r})\hat{\tau}(\boldsymbol{r})-\hat{\boldsymbol{j}}^2(\boldsymbol{r})\right\}+B_4\left\{\sum_q\hat{\rho}_q(\boldsymbol{r})\hat{\tau}_q(\boldsymbol{r})-\hat{\boldsymbol{j}}_q^2(\boldsymbol{r})\right\}\right] \\ &\quad -\int d\boldsymbol{r}\left[B_5\nabla\hat{\rho}(\boldsymbol{r})\nabla\hat{\rho}(\boldsymbol{r})+\sum_q B_6\nabla\hat{\rho}_q(\boldsymbol{r})\nabla\hat{\rho}_q(\boldsymbol{r})\right] \\ &\quad +\int d\boldsymbol{r}\left[B_1\hat{\rho}^2(\boldsymbol{r})+\sum_q B_2\hat{\rho}_q^2(\boldsymbol{r})\right]\end{aligned}$$

where the current density operator can be defined as

$$\hat{\boldsymbol{j}}(\boldsymbol{r})=\frac{1}{2i}\left(\psi^\dagger(\boldsymbol{r})\nabla\psi(\boldsymbol{r})-\nabla\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r})\right)$$

To calculate the double commutator relation, one prepares the commutator relations for each operators.

$$\begin{aligned}&[\hat{\rho}(\boldsymbol{r}),\hat{\rho}(\boldsymbol{r}')]=0 \\ &[\hat{\tau}(\boldsymbol{r}),\hat{\rho}(\boldsymbol{r}')]=\nabla\delta(\boldsymbol{r}-\boldsymbol{r}')\left(\nabla\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}')-\psi^\dagger(\boldsymbol{r}')\nabla\psi(\boldsymbol{r})\right) \\ &\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat{\rho}(\boldsymbol{r}')\right]=\frac{1}{2i}\left[\nabla\delta(\boldsymbol{r}-\boldsymbol{r}')\left(\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}')+\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r})\right)-\delta(\boldsymbol{r}-\boldsymbol{r}')\left(\psi^\dagger(\boldsymbol{r}')\nabla\psi(\boldsymbol{r})+\nabla\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}')\right)\right] \\ &[\nabla\hat{\rho}(\boldsymbol{r}),\hat{\rho}(\boldsymbol{r}')]=0\end{aligned}$$

Further here one calculates the double commutator relation for the non-zero commutator relations.

$$\begin{aligned}[\hat{\rho}(\boldsymbol{r}''),[\hat{\tau}(\boldsymbol{r}),\hat{\rho}(\boldsymbol{r}')]] &= \nabla\delta(\boldsymbol{r}-\boldsymbol{r}')\Big[\nabla\delta(\boldsymbol{r}-\boldsymbol{r}'')\left(\psi^\dagger(\boldsymbol{r}'')\psi(\boldsymbol{r}')+\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r}'')\right) \\ &\qquad -\delta(\boldsymbol{r}'-\boldsymbol{r}'')\left(\nabla\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}'')+\psi^\dagger(\boldsymbol{r}'')\nabla\psi(\boldsymbol{r})\right)\Big] \\ \left[\hat{\rho}(\boldsymbol{r}''),\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat{\rho}(\boldsymbol{r}')\right]\right] &= -\frac{1}{2i}\Big[\delta(\boldsymbol{r}-\boldsymbol{r}')\Big\{\delta(\boldsymbol{r}'-\boldsymbol{r}'')\left(\psi^\dagger(\boldsymbol{r}'')\nabla\psi(\boldsymbol{r})-\nabla\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}'')\right) \\ &\qquad -\nabla\delta(\boldsymbol{r}-\boldsymbol{r}'')\left(\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r}'')-\psi^\dagger(\boldsymbol{r}'')\psi(\boldsymbol{r}')\right)\Big\}\Big]\end{aligned}$$

And if one uses the relation as following,

$$[A,[BC,D]] = [A,B]\,[C,D] + B\,[A,[C,D]] + [A,[B,D]]\,C + [B,D]\,[A,C]$$

one can get

$$\begin{aligned}
\langle 0|\,[\hat\rho(\boldsymbol{r}''),[\hat\rho(\boldsymbol{r})\hat\tau(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')]]\,|0\rangle &= \langle 0|\hat\rho(\boldsymbol{r})\,[\hat\rho(\boldsymbol{r}''),[\hat\tau(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')]]\,|0\rangle \\
&= 2\nabla\delta(\boldsymbol{r}-\boldsymbol{r}')\nabla\delta(\boldsymbol{r}-\boldsymbol{r}'')\left(\rho(\boldsymbol{r})\rho(\boldsymbol{r}',\boldsymbol{r}'')-\rho(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}'',\boldsymbol{r})\right) \\
&\qquad -\delta(\boldsymbol{r}'-\boldsymbol{r}'')\nabla\delta(\boldsymbol{r}-\boldsymbol{r}')\left(2\rho(\boldsymbol{r})\nabla\rho(\boldsymbol{r},\boldsymbol{r}'')-\rho(\boldsymbol{r},\boldsymbol{r}'')\nabla\rho(\boldsymbol{r})\right)
\end{aligned}$$

$$\begin{aligned}
\langle 0|\left[\hat\rho(\boldsymbol{r}''),\left[\hat{\boldsymbol{j}}^2(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')\right]\right]|0\rangle &= \langle 0|\Big\{\hat{\boldsymbol{j}}(\boldsymbol{r})\cdot\left[\hat\rho(\boldsymbol{r}''),\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')\right]\right]+\left[\hat\rho(\boldsymbol{r}''),\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')\right]\right]\cdot\hat{\boldsymbol{j}}(\boldsymbol{r}) \\
&\qquad -\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')\right]\cdot\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat\rho(\boldsymbol{r}'')\right]-\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat\rho(\boldsymbol{r}'')\right]\cdot\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')\right]\Big\}|0\rangle \\
&= \Big[\nabla\delta(\boldsymbol{r}-\boldsymbol{r}')\cdot\nabla\delta(\boldsymbol{r}-\boldsymbol{r}'')\left(\rho(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r},\boldsymbol{r}'')-\rho(\boldsymbol{r})\rho(\boldsymbol{r}',\boldsymbol{r}'')\right) \\
&\qquad \frac{1}{2}\nabla\left(\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(\boldsymbol{r}-\boldsymbol{r}'')\right)\rho(\boldsymbol{r}',\boldsymbol{r}'')\nabla\rho(\boldsymbol{r}) \\
&\qquad -\delta(\boldsymbol{r}-\boldsymbol{r}'')\nabla\delta(\boldsymbol{r}-\boldsymbol{r}') \\
&\qquad\quad \times\Big(2\rho(\boldsymbol{r},\boldsymbol{r}')\nabla\rho(\boldsymbol{r},\boldsymbol{r}'')-\rho(\boldsymbol{r},\boldsymbol{r}'')\nabla\rho(\boldsymbol{r},\boldsymbol{r}')\Big) \\
&\qquad -\delta(\boldsymbol{r}-\boldsymbol{r}')\nabla\delta(\boldsymbol{r}-\boldsymbol{r}'') \\
&\qquad\quad \times\Big(2\rho(\boldsymbol{r},\boldsymbol{r}'')\nabla\rho(\boldsymbol{r},\boldsymbol{r}')-\rho(\boldsymbol{r},\boldsymbol{r}')\nabla\rho(\boldsymbol{r},\boldsymbol{r}'')\Big)\Big]
\end{aligned}$$

where

$$\begin{aligned}
\langle 0|\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')\right]\cdot\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat\rho(\boldsymbol{r}'')\right]|0\rangle &= -\frac{1}{2}\Big[\nabla\delta(\boldsymbol{r}-\boldsymbol{r}')\cdot\nabla\delta(\boldsymbol{r}-\boldsymbol{r}'')\left(\rho(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r},\boldsymbol{r}'')-\rho(\boldsymbol{r})\rho(\boldsymbol{r}',\boldsymbol{r}'')\right) \\
&\qquad +\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(\boldsymbol{r}-\boldsymbol{r}'')\left((\frac{1}{4}\nabla\rho(\boldsymbol{r}))^2-\rho(\boldsymbol{r})\tau(\boldsymbol{r})\right) \\
&\qquad -\delta(\boldsymbol{r}-\boldsymbol{r}'')\nabla\delta(\boldsymbol{r}-\boldsymbol{r}') \\
&\qquad\quad \times\Big(\rho(\boldsymbol{r},\boldsymbol{r}')\nabla\rho(\boldsymbol{r},\boldsymbol{r}'')-\frac{1}{2}\rho(\boldsymbol{r}',\boldsymbol{r}'')\nabla\rho(\boldsymbol{r}) \\
&\qquad\qquad +\rho(\boldsymbol{r},\boldsymbol{r}')\nabla\rho(\boldsymbol{r},\boldsymbol{r}'')-\rho(\boldsymbol{r},\boldsymbol{r}'')\nabla\rho(\boldsymbol{r},\boldsymbol{r}')\Big) \\
&\qquad -\delta(\boldsymbol{r}-\boldsymbol{r}')\nabla\delta(\boldsymbol{r}-\boldsymbol{r}'') \\
&\qquad\quad \times\Big(\rho(\boldsymbol{r},\boldsymbol{r}'')\nabla\rho(\boldsymbol{r},\boldsymbol{r}')-\frac{1}{2}\rho(\boldsymbol{r}'',\boldsymbol{r}')\nabla\rho(\boldsymbol{r}) \\
&\qquad\qquad +\rho(\boldsymbol{r},\boldsymbol{r}'')\nabla\rho(\boldsymbol{r},\boldsymbol{r}')-\rho(\boldsymbol{r},\boldsymbol{r}')\nabla\rho(\boldsymbol{r},\boldsymbol{r}'')\Big)\Big] \\
&= \langle 0|\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat\rho(\boldsymbol{r}'')\right]\cdot\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')\right]|0\rangle
\end{aligned}$$

$$\begin{aligned}
\langle 0|\hat{\boldsymbol{j}}(\boldsymbol{r})\cdot\left[\hat\rho(\boldsymbol{r}''),\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')\right]\right]|0\rangle &= \frac{1}{2}\Big[\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(\boldsymbol{r}'-\boldsymbol{r}'')\left(\tau(\boldsymbol{r})\rho(\boldsymbol{r})-\frac{1}{4}(\nabla\rho(\boldsymbol{r}))^2\right)\Big] \\
&= \langle 0|\left[\hat\rho(\boldsymbol{r}''),\left[\hat{\boldsymbol{j}}(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')\right]\right]\cdot\hat{\boldsymbol{j}}(\boldsymbol{r})|0\rangle
\end{aligned}$$

Then one can get the result

$$\iint d\boldsymbol{r}'d\boldsymbol{r}''f(\boldsymbol{r}'')\langle 0|\,[\hat\rho(\boldsymbol{r}''),[\hat\rho(\boldsymbol{r})\hat\tau(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')]]\,|0\rangle f(\boldsymbol{r}') = 0$$

$$\iint d\boldsymbol{r}'d\boldsymbol{r}''f(\boldsymbol{r}'')\langle 0|\left[\hat\rho(\boldsymbol{r}''),\left[\hat{\boldsymbol{j}}^2(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')\right]\right]|0\rangle f(\boldsymbol{r}') = f^2(\boldsymbol{r})\left(\rho(\boldsymbol{r})\tau(\boldsymbol{r})-\frac{1}{4}\left(\nabla\rho(\boldsymbol{r})\right)^2\right)$$

$$\iint d\boldsymbol{r}'d\boldsymbol{r}''f(\boldsymbol{r}'')\langle 0|\left[\hat\rho(\boldsymbol{r}''),\left[\hat\rho(\boldsymbol{r})\hat\tau(\boldsymbol{r})-\hat{\boldsymbol{j}}^2(\boldsymbol{r}),\hat\rho(\boldsymbol{r}')\right]\right]|0\rangle f(\boldsymbol{r}') = f^2(\boldsymbol{r})\left(\frac{1}{4}\left(\nabla\rho(\boldsymbol{r})\right)^2-\rho(\boldsymbol{r})\tau(\boldsymbol{r})\right)$$

Appendix C

Matrix element of the operator in the spherical symmetry

C.1 Spherical harmonics case

Scalar operator includes the Spherical harminics can be expressed as

$$\hat{Q}(\boldsymbol{r}) = \hat{Q}_L(r)\mathrm{Y}_{LM}(\hat{\boldsymbol{r}})$$

Matrix element of this operator can be obtained by the Wigner-Eckart theorem,

$$\begin{aligned}
\langle n'l'j'm'|\hat{Q}|nljm\rangle &= \sum_\sigma \int d\boldsymbol{r}\phi^*_{n'l'j'm'}(\boldsymbol{r}\sigma)\hat{Q}_L(r)\mathrm{Y}_{LM}(\hat{\boldsymbol{r}})\phi_{nljm}(\boldsymbol{r}\sigma) \\
&= (-)^{j'-m'}\begin{pmatrix} j' & L & j \\ -m' & M & m \end{pmatrix}\langle l'j'||\mathrm{Y}_L||lj\rangle \int r^2 dr \left[\frac{\phi^*_{n'l'j'}(r)}{r}\hat{Q}_L(r)\frac{\phi_{nlj}(r)}{r}\right]
\end{aligned}$$

In the case that $\hat{Q}(r)$ is the deribative operator for a radial coordinate, $\hat{Q}(r)$ operates only in [...]. For example, in the case of lapracian *i.e.* $\hat{Q}_L(r) = \Delta = \frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{\hat{\boldsymbol{L}}^2}{r^2}$

$$\begin{aligned}
\int r^2 dr \left[\frac{\phi^*_{n'l'j'}(r)}{r}\Delta\frac{\phi_{nlj}(r)}{r}\right] &= \int r^2 dr \left[\frac{\phi^*_{n'l'j'}(r)}{r}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{\hat{\boldsymbol{L}}^2}{r^2}\right)\frac{\phi_{nlj}(r)}{r}\right] \\
&= \int dr \left[\phi^*_{n'l'j'}(r)\left(\frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2}\right)\phi_{nlj}(r)\right]
\end{aligned}$$

The complex conjugate of this can be expressed as

$$\begin{aligned}
\langle nljm|\hat{Q}^*|n'l'j'm'\rangle &= \sum_\sigma \int d\boldsymbol{r}\phi^*_{nljm}(\boldsymbol{r}\sigma)\hat{Q}_L(r)\mathrm{Y}^*_{LM}(\hat{\boldsymbol{r}})\phi_{n'l'j'm'}(\boldsymbol{r}\sigma) \\
&= (-)^M \sum_\sigma \int d\boldsymbol{r}\phi^*_{nljm}(\boldsymbol{r}\sigma)\hat{Q}_L(r)\mathrm{Y}_{L-M}(\hat{\boldsymbol{r}})\phi_{n'l'j'm'}(\boldsymbol{r}\sigma) \\
&= (-)^{j-m+M}\begin{pmatrix} j & L & j' \\ -m & -M & m' \end{pmatrix}\langle lj||\mathrm{Y}_L||l'j'\rangle \int r^2 dr \left[\frac{\phi^*_{nlj}(r)}{r}\hat{Q}_L(r)\frac{\phi_{n'l'j'}(r)}{r}\right] \\
&= (-)^{j-m'}\begin{pmatrix} j' & L & j \\ -m' & M & m \end{pmatrix}\langle lj||\mathrm{Y}_L||l'j'\rangle \int r^2 dr \left[\frac{\phi^*_{nlj}(r)}{r}\hat{Q}_L(r)\frac{\phi_{n'l'j'}(r)}{r}\right]
\end{aligned}$$

where we used the 3-j symbol's property, $-m' + M + m = 0$, and M is integer.

$$(-)^{j-m+M} = (-)^{j-m-M} = (-)^{j-m'}$$

Now we calculates the quantity

$$\sum_{nljm}\sum_{n'l'j'm'}\langle nljm|\hat{Q}^*|n'l'j'm'\rangle\langle n'l'j'm'|\hat{Q}|nljm\rangle$$

$$= \sum_{nljm}\sum_{n'l'j'm'}(-)^{j+j'-2m'}\begin{pmatrix} j' & L & j \\ -m' & M & m \end{pmatrix}^2 \langle lj||\mathrm{Y}_L||l'j'\rangle\langle l'j'||\mathrm{Y}_L||lj\rangle$$

$$\times \int r'^2dr'\left[\frac{\phi^*_{nlj}(r')}{r'}\hat{Q}_L(r')\frac{\phi_{n'l'j'}(r')}{r'}\right]\int r^2dr\left[\frac{\phi^*_{n'l'j'}(r)}{r}\hat{Q}_L(r)\frac{\phi_{nlj}(r)}{r}\right]$$

$$= \sum_{nlj}\sum_{n'l'j'}\frac{(-)^{j-j'}}{2L+1}\langle lj||\mathrm{Y}_L||l'j'\rangle\langle l'j'||\mathrm{Y}_L||lj\rangle$$

$$\times \int r'^2dr'\left[\frac{\phi^*_{nlj}(r')}{r'}\hat{Q}_L(r')\frac{\phi_{n'l'j'}(r')}{r'}\right]\int r^2dr\left[\frac{\phi^*_{n'l'j'}(r)}{r}\hat{Q}_L(r)\frac{\phi_{nlj}(r)}{r}\right]$$

where we used

$$(-)^{2m} = (-)^{2m_l}(-)^{\pm 1} = -1$$
$$(-)^{2j'} = (-)^{2l'\pm 1} = -1 \rightarrow (-)^{j'-1} = (-)^{-j'}$$
then
$$(-)^{j+j'-2m'} = (-)^{j+j'-1} = (-)^{j-j'}$$

And also

$$\sum_{mm'}\begin{pmatrix} j' & L & j \\ -m' & M & m \end{pmatrix}^2 = \frac{1}{2L+1}$$

C.2 Matrix elements of the tensor operators

A matrix element is given by

$$\begin{aligned}
\langle l'm'_l|Y_{LM}|lm_l\rangle &= \int d\hat{\boldsymbol{r}}Y^*_{l'm'_l}(\hat{\boldsymbol{r}})Y_{LM}(\hat{\boldsymbol{r}})Y_{lm_l}(\hat{\boldsymbol{r}}) \\
&= \sqrt{\frac{(2L+1)(2l'+1)}{4\pi(2l+1)}}\langle L0:l0|l'0\rangle\langle LM:lm_l|l'm'_l\rangle \\
&= (-)^{m_l}\sqrt{\frac{(2L+1)(2l+1)(2l'+1)}{4\pi}}\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} L & l & l' \\ M & m_l & -m'_l \end{pmatrix},
\end{aligned}$$

on the other hand, Wigner-Eckart's theorem gives

$$\langle l'm'_l|Y_{LM}|lm_l\rangle = (-)^{l'-m'_l}\begin{pmatrix} l' & L & l \\ -m'_l & M & m_l \end{pmatrix}\langle l'||Y_L||l\rangle$$

where $\langle||\cdots||\rangle$ means a reduced matrix element. Then one can get

$$\langle l'||Y_L||l\rangle = (-)^{l'}\sqrt{\frac{(2L+1)(2l+1)(2l'+1)}{4\pi}}\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}$$

and using the relation

$$\begin{aligned}
\langle l'j'||Y_L||lj\rangle &= (-)^{j+l'+L+\frac{1}{2}}(2j+1)^{\frac{1}{2}}(2j'+1)^{\frac{1}{2}}\begin{Bmatrix} j' & l' & \frac{1}{2} \\ l & j & L \end{Bmatrix}\langle l'||Y_L||l\rangle \qquad \text{gives} \\
&= (-)^{j+L+\frac{1}{2}}\sqrt{\frac{(2L+1)(2l+1)(2l'+1)(2j+1)(2j'+1)}{4\pi}}\begin{Bmatrix} j' & l' & \frac{1}{2} \\ l & j & L \end{Bmatrix}\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

From the property of the 6j, 3j symbol,

$$\left\{ \begin{array}{ccc} j' & l' & \frac{1}{2} \\ l & j & L \end{array} \right\} \left(\begin{array}{ccc} L & l & l' \\ 0 & 0 & 0 \end{array} \right) = \frac{(-)^{j+j'}\left(1+(-)^{L+l+l'}\right)}{\sqrt{(2L+1)(2l+1)(2l'+1)}} \langle j1/2; j'-1/2|L0\rangle\rangle$$

one can get

$$\begin{aligned} \langle l'j'||Y_L||lj\rangle &= (-)^{j'+L-\frac{1}{2}}\left(1+(-)^{L+l+l'}\right)\sqrt{\frac{(2j+1)(2j'+1)}{16\pi}}\langle j1/2; j'-1/2|L0\rangle \\ &= (-)^{j-j'+L}\left(1+(-)^{L+l+l'}\right)\sqrt{\frac{(2j+1)(2L+1)}{16\pi}}\langle j1/2; L0|j'1/2\rangle \end{aligned}$$

C.2.1 ∇ and angular momentum

The goal is the derivation of

$$\langle l'j'||\boldsymbol{Y}_{L\lambda}\cdot\nabla||lj\rangle$$

by using

$$\nabla = \hat{\boldsymbol{r}}\frac{\partial}{\partial r} - i\frac{\boldsymbol{r}\times\boldsymbol{L}}{r^2}$$

C.2.2 $\langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot\nabla|lm\rangle$

$$\begin{aligned} \langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot\nabla|lm\rangle &= \int d\hat{\boldsymbol{r}}Y^*_{l'm'}(\hat{\boldsymbol{r}})\boldsymbol{Y}_{L\lambda M}(\hat{\boldsymbol{r}})\cdot\left(\hat{\boldsymbol{r}}\frac{\partial}{\partial r} - i\frac{\boldsymbol{r}\times\boldsymbol{L}}{r^2}\right)Y_{lm}(\hat{\boldsymbol{r}}) \\ &= \left[\int d\hat{\boldsymbol{r}}Y^*_{l'm'}(\hat{\boldsymbol{r}})\boldsymbol{Y}_{L\lambda M}(\hat{\boldsymbol{r}})\cdot\underline{\hat{\boldsymbol{r}}Y_{lm}(\hat{\boldsymbol{r}})}\right]\frac{\partial}{\partial r} - \left[\int d\hat{\boldsymbol{r}}Y^*_{l'm'}(\hat{\boldsymbol{r}})\boldsymbol{Y}_{L\lambda M}(\hat{\boldsymbol{r}})\cdot\underline{i\hat{\boldsymbol{r}}\times\boldsymbol{L}Y_{lm}(\hat{\boldsymbol{r}})}\right]\frac{1}{r} \end{aligned}$$

where one can apply basic formulae to underline parts

$$\begin{aligned} \hat{\boldsymbol{r}}Y_{lm}(\hat{\boldsymbol{r}}) &= -\sum_{\eta=l\pm1}\langle l0:10|\eta0\rangle\boldsymbol{Y}_{l\eta m}(\hat{\boldsymbol{r}}) \qquad \textit{(Rose p122 (6.32))} \\ &= -\left[\frac{l+1}{2l+1}\right]^{\frac{1}{2}}\boldsymbol{Y}_{ll+1m}(\hat{\boldsymbol{r}}) + \left[\frac{l}{2l+1}\right]^{\frac{1}{2}}\boldsymbol{Y}_{ll-1m}(\hat{\boldsymbol{r}}) \qquad \textit{(Edmonds p84 (5.9.16))} \\ i\hat{\boldsymbol{r}}\times\boldsymbol{L}Y_{lm}(\hat{\boldsymbol{r}}) &= [6l(l+1)(2l+1)]^{\frac{1}{2}}\sum_{\eta=l\pm1}\langle l0:10|\eta0\rangle W(l\eta11:1l)\boldsymbol{Y}_{l\eta m}(\hat{\boldsymbol{r}}) \qquad \textit{(Rose p123 (6.39))} \end{aligned}$$

$W(l\eta 11:1l)$ is the *Racah* coefficient

$$= -l\left[\frac{l+1}{2l+1}\right]^{\frac{1}{2}}\boldsymbol{Y}_{ll+1m}(\hat{\boldsymbol{r}}) - (l+1)\left[\frac{l}{2l+1}\right]^{\frac{1}{2}}\boldsymbol{Y}_{ll-1m}(\hat{\boldsymbol{r}})$$

Then one can get the result

$$\begin{aligned} \langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot\nabla|lm\rangle &= -\left[\frac{l+1}{2l+1}\right]^{\frac{1}{2}}\left[\int d\hat{\boldsymbol{r}}Y^*_{l'm'}(\hat{\boldsymbol{r}})\boldsymbol{Y}_{L\lambda M}(\hat{\boldsymbol{r}})\cdot\boldsymbol{Y}_{ll+1m}(\hat{\boldsymbol{r}})\right]\left(\frac{\partial}{\partial r} - \frac{l}{r}\right) \\ &\quad + \left[\frac{l}{2l+1}\right]^{\frac{1}{2}}\left[\int d\hat{\boldsymbol{r}}Y^*_{l'm'}(\hat{\boldsymbol{r}})\boldsymbol{Y}_{L\lambda M}(\hat{\boldsymbol{r}})\cdot\boldsymbol{Y}_{ll-1m}(\hat{\boldsymbol{r}})\right]\left(\frac{\partial}{\partial r} + \frac{l+1}{r}\right) \end{aligned}$$

One can give the explicit expression of $\left[\int d\hat{\boldsymbol{r}}Y^*_{l'm'}(\hat{\boldsymbol{r}})\boldsymbol{Y}_{L\lambda M}(\hat{\boldsymbol{r}})\cdot\boldsymbol{Y}_{ll''m}(\hat{\boldsymbol{r}})\right]$ by using the definition of $\boldsymbol{Y}$ as

$$\begin{aligned} \int d\hat{\boldsymbol{r}}Y^*_{l'm'}(\hat{\boldsymbol{r}})\boldsymbol{Y}_{L\lambda M}(\hat{\boldsymbol{r}})\cdot\boldsymbol{Y}_{ll''m}(\hat{\boldsymbol{r}}) &= (-)^{1+m+M}\left[\frac{(2l+1)(2l'+1)(2L+1)(2\lambda+1)(2l''+1)}{4\pi}\right]^{\frac{1}{2}} \\ &\quad \times\left(\begin{array}{ccc} l' & \lambda & l'' \\ 0 & 0 & 0 \end{array}\right)\left\{\begin{array}{ccc} L & l & l' \\ l'' & \lambda & 1 \end{array}\right\}\left(\begin{array}{ccc} L & l & l' \\ M & m & -m' \end{array}\right) \end{aligned}$$

From the Wigner-Eckart's theorem,

$$\langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot\nabla|lm\rangle = (-)^{l'-m'}\begin{pmatrix} l' & L & l \\ -m' & M & m \end{pmatrix}\langle l'||\boldsymbol{Y}_{L\lambda}\cdot\nabla||l\rangle$$

one can get $\langle l'||\boldsymbol{Y}\cdot\nabla||l\rangle$.

$$\begin{aligned}
\langle l'||\boldsymbol{Y}_{L\lambda}\cdot\nabla||l\rangle &= (-)^{l'+1}\left[\frac{(2l'+1)(2L+1)(2\lambda+1)}{4\pi}\right]^{\frac{1}{2}} \\
&\quad\times\Bigg\{\underline{[(2l-1)l]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l-1 \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} L & l & l' \\ l-1 & \lambda & 1 \end{Bmatrix}}\left(\frac{\partial}{\partial r}+\frac{l+1}{r}\right) \\
&\qquad -[(2l+3)(l+1)]^{\frac{1}{2}}\underline{\begin{pmatrix} l' & \lambda & l+1 \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} L & l & l' \\ l+1 & \lambda & 1 \end{Bmatrix}}\left(\frac{\partial}{\partial r}-\frac{l}{r}\right)\Bigg\} \\
&= (-)^{l'+1}\left[\frac{(2l'+1)(2L+1)(2\lambda+1)}{4\pi}\right]^{\frac{1}{2}} \\
&\quad\times\Bigg\{\underline{[(2l-1)l]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l-1 \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} l' & \lambda & l-1 \\ 1 & l & L \end{Bmatrix}}\left(\frac{\partial}{\partial r}+\frac{l+1}{r}\right) \\
&\qquad \underline{-[(2l+3)(l+1)]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l+1 \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} l' & \lambda & l+1 \\ 1 & l & L \end{Bmatrix}}\left(\frac{\partial}{\partial r}-\frac{l}{r}\right)\Bigg\}
\end{aligned}$$

Applying the properties of the 3-j symbol and 6-j symbol, underline parts can be re-written as

$$\begin{aligned}
&[(2l-1)l]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l-1 \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} l' & \lambda & l-1 \\ 1 & l & L \end{Bmatrix} \\
&= [(2l-1)l]^{\frac{1}{2}}\Big\{2(-)^{l+L}\begin{pmatrix} l' & l & L \\ 0 & 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & \lambda & L \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & l & l-1 \\ -1 & 1 & 0 \end{pmatrix} \\
&\qquad +(-)^{l+L+1}\begin{pmatrix} l' & l & L \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & \lambda & L \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l & l-1 \\ 0 & 0 & 0 \end{pmatrix}\Big\} \\
= &\sqrt{\frac{1}{2(2L+1)(2\lambda+1)}} \\
&\times\left\{\sqrt{\frac{(3L-\lambda+1)l(l+1)}{(2l+1)}}\begin{pmatrix} l' & l & L \\ 0 & 1 & -1 \end{pmatrix}+(-)^{L+1}(-)^{\frac{1}{2}(\lambda+L+1)}l\sqrt{\frac{(\lambda+L+1)}{(2l+1)}}\begin{pmatrix} l' & l & L \\ 0 & 0 & 0 \end{pmatrix}\right\}
\end{aligned}$$

$$
\begin{aligned}
&[(2l+3)(l+1)]^{\frac{1}{2}} \begin{pmatrix} l' & \lambda & l+1 \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l' & \lambda & l+1 \\ 1 & l & L \end{Bmatrix} \\
&= [(2l+3)(l+1)]^{\frac{1}{2}} \Big\{ 2(-)^{l+L} \begin{pmatrix} l' & l & L \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & \lambda & L \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & l & l+1 \\ -1 & 1 & 0 \end{pmatrix} \\
&\qquad + (-)^{l+L+1} \begin{pmatrix} l' & l & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & \lambda & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l & l+1 \\ 0 & 0 & 0 \end{pmatrix} \Big\} \\
&= \sqrt{\frac{1}{2(2L+1)(2\lambda+1)}} \\
&\qquad \times \left\{ \sqrt{\frac{l(l+1)(3L-\lambda+1)}{(2l+1)}} \begin{pmatrix} l' & l & L \\ 0 & 1 & -1 \end{pmatrix} + (-)^{L} (-)^{\frac{1}{2}(\lambda+L+1)} (l+1) \sqrt{\frac{(\lambda+L+1)}{(2l+1)}} \begin{pmatrix} l' & l & L \\ 0 & 0 & 0 \end{pmatrix} \right\}
\end{aligned}
$$

Then one can get

$$
\begin{aligned}
&\langle l' || \boldsymbol{Y}_{L\lambda} \cdot \nabla || l \rangle \\
&= (-)^{l'+1} \left[\frac{(2l'+1)}{8\pi} \right]^{\frac{1}{2}} \\
&\times \Big\{ \left[\sqrt{\frac{(3L-\lambda+1)l(l+1)}{(2l+1)}} \begin{pmatrix} l' & l & L \\ 0 & 1 & -1 \end{pmatrix} + (-)^{L+1} (-)^{\frac{1}{2}(\lambda+L+1)} l \sqrt{\frac{(\lambda+L+1)}{(2l+1)}} \begin{pmatrix} l' & l & L \\ 0 & 0 & 0 \end{pmatrix} \right] \left(\frac{\partial}{\partial r} + \frac{l+1}{r} \right) \\
&- \left[\sqrt{\frac{l(l+1)(3L-\lambda+1)}{(2l+1)}} \begin{pmatrix} l' & l & L \\ 0 & 1 & -1 \end{pmatrix} + (-)^{L} (-)^{\frac{1}{2}(\lambda+L+1)} (l+1) \sqrt{\frac{(\lambda+L+1)}{(2l+1)}} \begin{pmatrix} l' & l & L \\ 0 & 0 & 0 \end{pmatrix} \right] \left(\frac{\partial}{\partial r} - \frac{l}{r} \right) \Big\} \\
&= (-)^{l'+1} \left[\frac{(2l'+1)(2l+1)}{8\pi} \right]^{\frac{1}{2}} \\
&\times \left[(-)^{L+1} (-)^{\frac{1}{2}(\lambda+L+1)} \sqrt{(\lambda+L+1)} \begin{pmatrix} l' & l & L \\ 0 & 0 & 0 \end{pmatrix} \frac{\partial}{\partial r} + \sqrt{l(l+1)(3L-\lambda+1)} \begin{pmatrix} l' & l & L \\ 0 & 1 & -1 \end{pmatrix} \frac{1}{r} \right]
\end{aligned}
$$

Next one can apply below formulae

$$
\begin{aligned}
\begin{Bmatrix} j' & l' & \frac{1}{2} \\ l & j & L \end{Bmatrix} \begin{pmatrix} l' & l & L \\ 0 & 0 & 0 \end{pmatrix} &= (-)^{j+j'} \left(1 + (-)^{L+l+l'}\right) \begin{pmatrix} l' & j' & \frac{1}{2} \\ 0 & \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} j & l & \frac{1}{2} \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} j & j' & L \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \\
&= \frac{(-)^{l+l'+1} \left(1 + (-)^{L+l+l'}\right)}{\sqrt{(2L+1)(2j+1)(2j'+1)}} \langle l'0 : \frac{1}{2}\frac{1}{2} | j'\frac{1}{2} \rangle \langle l0 : \frac{1}{2}\frac{1}{2} | j\frac{1}{2} \rangle \langle j\frac{1}{2} : j' - \frac{1}{2} | L0 \rangle \\
&= \frac{(-)^{j+j'} \left(1 + (-)^{L+l+l'}\right)}{\sqrt{(2L+1)(2l+1)(2l'+1)}} \langle j\frac{1}{2} : j' - \frac{1}{2} | L0 \rangle
\end{aligned}
$$

$$
\begin{aligned}
\begin{Bmatrix} j' & l' & \frac{1}{2} \\ l & j & L \end{Bmatrix} \begin{pmatrix} l' & l & L \\ 0 & 1 & -1 \end{pmatrix} &= (-)^{j+j'} \begin{pmatrix} l' & j' & \frac{1}{2} \\ 0 & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} j & l & \frac{1}{2} \\ -\frac{1}{2} & 1 & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} j & j' & L \\ \frac{1}{2} & \frac{1}{2} & -1 \end{pmatrix} \\
&\quad + (-)^{j+j'+1} \begin{pmatrix} l' & j' & \frac{1}{2} \\ 0 & \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} j & l & \frac{1}{2} \\ -\frac{3}{2} & 1 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} j & j' & L \\ \frac{3}{2} & -\frac{1}{2} & -1 \end{pmatrix} \\
&= \frac{1}{\sqrt{2(2L+1)(2j+1)(2l+1)(2l'+1)}} \\
&\quad \times \left\{ (-)^{l+l'+1} \sqrt{2l - j + \frac{1}{2}} \langle j\frac{1}{2} : j'\frac{1}{2} | L1 \rangle + (-)^{j+j'+1} \sqrt{3j - 2l + \frac{1}{2}} \langle j\frac{3}{2} : j' - \frac{1}{2} | L1 \rangle \right\}
\end{aligned}
$$

where

$$
\langle l'0 : \frac{1}{2}\frac{1}{2} | j'\frac{1}{2} \rangle = (-)^{l'-j'+\frac{1}{2}} \sqrt{\frac{j'+\frac{1}{2}}{2l'+1}} \qquad \langle l0 : \frac{1}{2}\frac{1}{2} | j\frac{1}{2} \rangle = (-)^{l-j+\frac{1}{2}} \sqrt{\frac{j+\frac{1}{2}}{2l+1}}
$$

$$\langle l1:\frac{1}{2}-\frac{1}{2}|j\frac{1}{2}\rangle=\sqrt{\frac{2l-j+\frac{1}{2}}{2l+1}}\qquad\langle l1:\frac{1}{2}\frac{1}{2}|j\frac{3}{2}\rangle=(-)^{l-j+\frac{1}{2}}\sqrt{\frac{3j-2l+\frac{1}{2}}{2l+1}}$$

C.2.3 Summary

Then one can get $\langle l'j'||\boldsymbol{Y}_{L\lambda}\cdot\nabla||lj\rangle$

$$\begin{aligned}\langle l'j'||\boldsymbol{Y}_{L\lambda}\cdot\nabla||lj\rangle &= (-)^{j+l'+L+\frac{1}{2}}(2j+1)^{\frac{1}{2}}(2j'+1)^{\frac{1}{2}}\left\{\begin{array}{ccc} j' & l' & \frac{1}{2}\\ l & j & L\end{array}\right\}\langle l'||\boldsymbol{Y}_{L\lambda}\cdot\nabla||l\rangle\\ &= F^{L\lambda}_{l'j'lj}\frac{\partial}{\partial r}+G^{L\lambda}_{l'j'lj}\frac{1}{r}\end{aligned}$$

$$\begin{aligned}F^{L\lambda}_{l'j'lj} &= (-)^{j+\frac{1}{2}}(-)^{\frac{1}{2}(\lambda+L+1)}\left[\frac{(2l'+1)(2l+1)(2j+1)(2j'+1)}{8\pi}\right]^{\frac{1}{2}}\sqrt{(\lambda+L+1)}\left\{\begin{array}{ccc} j' & l' & \frac{1}{2}\\ l & j & L\end{array}\right\}\left(\begin{array}{ccc} l' & l & L\\ 0 & 0 & 0\end{array}\right)\\ &= (-)^{j'-\frac{1}{2}}(-)^{\frac{1}{2}(\lambda+L+1)}\left[\frac{(2j'+1)(2j+1)}{(2L+1)}\right]^{\frac{1}{2}}\sqrt{\frac{(\lambda+L+1)}{8\pi}}\langle j\frac{1}{2}:j'-\frac{1}{2}|L0\rangle\\ G^{L\lambda}_{l'j'lj} &= (-)^{j+L-\frac{1}{2}}\left[\frac{(2j+1)(2j'+1)(2l'+1)(2l+1)}{8\pi}\right]^{\frac{1}{2}}\sqrt{l(l+1)(3L-\lambda+1)}\left\{\begin{array}{ccc} j' & l' & \frac{1}{2}\\ l & j & L\end{array}\right\}\left(\begin{array}{ccc} l' & l & L\\ 0 & 1 & -1\end{array}\right)\\ &= (-)^{j-\frac{1}{2}+L}\sqrt{\frac{l(l+1)(2j'+1)(3L-\lambda+1)}{16\pi(2L+1)}}\\ &\quad\times\left\{(-)^{l+l'+1}\sqrt{2(l-j)+j+\frac{1}{2}}\langle j\frac{1}{2}:j'\frac{1}{2}|L1\rangle+(-)^{j+j'+1}\sqrt{2(j-l)+j+\frac{1}{2}}\langle j\frac{3}{2}:j'-\frac{1}{2}|L1\rangle\right\}\end{aligned}$$

Symmetry of these coefficients

$$\begin{aligned}F^{L\lambda}_{ljl'j'} &= (-)^{j-\frac{1}{2}}(-)^{\frac{1}{2}(\lambda+L+1)}\left[\frac{(2j'+1)(2j+1)}{(2L+1)}\right]^{\frac{1}{2}}\sqrt{\frac{(\lambda+L+1)}{8\pi}}\langle j'\frac{1}{2}:j-\frac{1}{2}|L0\rangle\\ &= (-)^{j-\frac{1}{2}}(-)^{\frac{1}{2}(\lambda+L+1)}\left[\frac{(2j'+1)(2j+1)}{(2L+1)}\right]^{\frac{1}{2}}\sqrt{\frac{(\lambda+L+1)}{8\pi}}\langle j\frac{1}{2}:j'-\frac{1}{2}|L0\rangle\\ &= (-)^{j'-j}F^{L\lambda}_{l'j'lj}\end{aligned}$$

C.2.4 Application

The porpose of this section is to derive

$$\langle l'j'||\overleftarrow{\nabla}\cdot\boldsymbol{Y}_{L\lambda}\pm\boldsymbol{Y}_{L\lambda}\cdot\overrightarrow{\nabla}||lj\rangle,$$

by using $\langle l'j'||\boldsymbol{Y}_{L\lambda}\cdot\overrightarrow{\nabla}||lj\rangle$ shown in the previous section.

Starting point is

$$\begin{aligned}\langle l'j'm'|\overleftarrow{\nabla}\cdot\boldsymbol{Y}_{L\lambda M}|ljm\rangle &= \langle ljm|\boldsymbol{Y}^{*}_{L\lambda M}\cdot\overrightarrow{\nabla}|l'j'm'\rangle^{*}\\ &= (-)^{M}\langle ljm|\boldsymbol{Y}_{L\lambda -M}\cdot\overrightarrow{\nabla}|l'j'm'\rangle^{*}\\ &= (-)^{M}(-)^{j-m}\left(\begin{array}{ccc} j & L & j'\\ -m & -M & m'\end{array}\right)\langle lj||\boldsymbol{Y}_{L\lambda}\cdot\overrightarrow{\nabla}||l'j'\rangle^{*}\\ &= (-)^{M}(-)^{j-m}\left(\begin{array}{ccc} j' & L & j\\ -m' & M & m\end{array}\right)\langle lj||\boldsymbol{Y}_{L\lambda}\cdot\overrightarrow{\nabla}||l'j'\rangle^{*}\end{aligned}$$

Next one spplies the Wigner-Eckart's theorem to the right hand side,

$$\langle l'j'm'|\overleftarrow{\nabla}\cdot\boldsymbol{Y}_{L\lambda M}|ljm\rangle=(-)^{j'-m'}\left(\begin{array}{ccc} j' & L & j\\ -m' & M & m\end{array}\right)\langle l'j'||\overleftarrow{\nabla}\cdot\boldsymbol{Y}_{L\lambda}||lj\rangle$$

Then one can get

$$\begin{aligned}\langle l'j'||\overleftarrow{\nabla}\cdot\boldsymbol{Y}_{L\lambda}||lj\rangle &= (-)^{j-j'}\langle lj||\boldsymbol{Y}_{L\lambda}\cdot\overrightarrow{\nabla}||l'j'\rangle^* \\ &= (-)^{j-j'}\left[F^{L\lambda}_{ljl'j'}\frac{\partial}{\partial r}+G^{L\lambda}_{ljl'j'}\frac{1}{r}\right]^* = F^{L\lambda}_{l'j'lj}\frac{\overleftarrow{\partial}}{\partial r}+(-)^{j-j'}G^{L\lambda}_{ljl'j'}\frac{1}{r}\end{aligned}$$

Finally,

$$\begin{aligned}\langle l'j'||\overleftarrow{\nabla}\cdot\boldsymbol{Y}_{L\lambda}\pm\boldsymbol{Y}_{L\lambda}\cdot\overrightarrow{\nabla}||lj\rangle, &= \left(F^{L\lambda}_{l'j'lj}\frac{\overleftarrow{\partial}}{\partial r}+(-)^{j-j'}G^{L\lambda}_{ljl'j'}\frac{1}{r}\right)\pm\left(F^{L\lambda}_{l'j'lj}\frac{\overrightarrow{\partial}}{\partial r}+G^{L\lambda}_{l'j'lj}\frac{1}{r}\right) \\ &= F^{L\lambda}_{l'j'lj}\left(\frac{\overleftarrow{\partial}}{\partial r}\pm\frac{\overrightarrow{\partial}}{\partial r}\right)+\left((-)^{j-j'}G^{L\lambda}_{ljl'j'}\pm G^{L\lambda}_{l'j'lj}\right)\frac{1}{r}\end{aligned}$$

$$\begin{aligned}&(-)^{j-j'}G^{L\lambda}_{ljl'j'} \\ &= (-)^{j+L-\frac{1}{2}}\left[\frac{(2j+1)(2j'+1)(2l'+1)(2l+1)}{8\pi}\right]^{\frac{1}{2}}\sqrt{l'(l'+1)(3L-\lambda+1)}\left\{\begin{array}{ccc} j & l & \frac{1}{2}\\ l' & j' & L\end{array}\right\}\left(\begin{array}{ccc} l & l' & L\\ 0 & 1 & -1\end{array}\right) \\ &= (-)^{j+l+l'-\frac{1}{2}}\left[\frac{(2j+1)(2j'+1)(2l'+1)(2l+1)}{8\pi}\right]^{\frac{1}{2}}\sqrt{l'(l'+1)(3L-\lambda+1)}\left\{\begin{array}{ccc} j' & l' & \frac{1}{2}\\ l & j & L\end{array}\right\}\left(\begin{array}{ccc} l' & l & L\\ 1 & 0 & -1\end{array}\right) \\ &= (-)^{j+l+l'-\frac{1}{2}}\left[\frac{(2j+1)(2j'+1)(2l'+1)(2l+1)(3L-\lambda+1)}{8\pi}\right]^{\frac{1}{2}} \\ &\quad\times\left[\sqrt{L(L+1)}\left\{\begin{array}{ccc} j' & l' & \frac{1}{2}\\ l & j & L\end{array}\right\}\left(\begin{array}{ccc} l' & l & L\\ 0 & 0 & 0\end{array}\right)-\sqrt{l(l+1)}\left\{\begin{array}{ccc} j' & l' & \frac{1}{2}\\ l & j & L\end{array}\right\}\left(\begin{array}{ccc} l' & l & L\\ 0 & 1 & -1\end{array}\right)\right] \\ &= (-)^{\frac{1}{2}(3L+1-\lambda)}\sqrt{\frac{L(L+1)(3L-\lambda+1)}{\lambda+L+1}}F^{L\lambda}_{l'j'lj}-(-)^{L+l+l'}G^{L\lambda}_{l'j'lj} \\ &= (-)^{\frac{1}{2}(3L+1-\lambda)}\left[\frac{3L-\lambda+1}{2}\right]F^{L\lambda}_{l'j'lj}-(-)^{L+l+l'}G^{L\lambda}_{l'j'lj}\end{aligned}$$

Therefore

$$\begin{aligned}(-)^{j-j'}G^{L\lambda}_{ljl'j'}\pm G^{L\lambda}_{l'j'lj} &= (-)^{\frac{1}{2}(3L+1-\lambda)}\left[\frac{3L-\lambda+1}{2}\right]F^{L\lambda}_{l'j'lj}+((-)^{L+l+l'+1}\pm 1)G^{L\lambda}_{l'j'lj} \\ &\equiv K^{(\pm)L\lambda}_{l'j'lj}\end{aligned}$$

Symmetry of $K^{(\pm)L\lambda}_{l'j'lj}$

$$\begin{aligned}K^{(\pm)L\lambda}_{ljl'j'} &= (-)^{j-j'}G^{L\lambda}_{l'j'lj}\pm G^{L\lambda}_{ljl'j'} = \pm(-)^{j-j'}\left((-)^{j-j'}G^{L\lambda}_{ljl'j'}\pm G^{L\lambda}_{l'j'lj}\right) \\ &= \pm(-)^{j-j'}K^{(\pm)L\lambda}_{l'j'lj}\end{aligned}$$

C.2.5 Matrix element of $\langle l'j'||\nabla\cdot Y_L\nabla||lj\rangle$

$$\begin{aligned}\langle l'm'_l|\overleftarrow{\nabla}\cdot Y_{LM}\overrightarrow{\nabla}|lm_l\rangle &= (-)^{\frac{1}{2}(l+l')+1}\sum_{\eta=l\pm1}\sum_{\eta'=l'\pm1}\sqrt{\frac{(\eta'+l'+1)(\eta+l+1)}{4(2l+1)(2l'+1)}} \\ &\quad\times(-)^{\frac{1}{2}(\eta+\eta')}\int d\hat{\boldsymbol{r}}\left[\boldsymbol{Y}^*_{l'\eta'm'_l}(\hat{\boldsymbol{r}})\cdot Y_{LM}(\hat{\boldsymbol{r}})\boldsymbol{Y}_{l\eta m_l}(\hat{\boldsymbol{r}})\right] \\ &\quad\times\left[\left(\frac{\overleftarrow{\partial}}{\partial r}+(-)^{\frac{1}{2}(\eta'-l'-1)}\frac{3l'-\eta'+1}{2r}\right)\right]\left[\left(\frac{\overrightarrow{\partial}}{\partial r}+(-)^{\frac{1}{2}(\eta-l-1)}\frac{3l-\eta+1}{2r}\right)\right]\end{aligned}$$

where

$$
\begin{aligned}
\int d\hat{\boldsymbol{r}}\left[\boldsymbol{Y}^{*}_{l'\eta'm'_l}(\hat{\boldsymbol{r}})\cdot Y_{LM}(\hat{\boldsymbol{r}})\boldsymbol{Y}_{l\eta m_l}(\hat{\boldsymbol{r}})\right] &= (-)^{m'_l+1}\left[\frac{(2L+1)(2l+1)(2l'+1)(2\eta+1)(2\eta'+1)}{4\pi}\right]^{\frac{1}{2}} \\
&\times\begin{pmatrix} L & \eta' & \eta \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & l & L \\ \eta & \eta' & 1\end{Bmatrix}\begin{pmatrix} l' & l & L \\ -m'_l & m_l & M\end{pmatrix}
\end{aligned}
$$

On the other hand, Wigner-Eckart's theorem gives

$$
\begin{aligned}
\langle l'm'_l|\overleftarrow{\nabla}\cdot Y_{LM}\overrightarrow{\nabla}|lm_l\rangle &= (-)^{l'-m'_l}\begin{pmatrix} l' & L & l \\ -m'_l & M & m_l\end{pmatrix}\langle l'||\overleftarrow{\nabla}\cdot Y_L\overrightarrow{\nabla}||l\rangle \\
&= (-)^{L+l-m'_l}\begin{pmatrix} l' & l & L \\ -m'_l & m_l & M\end{pmatrix}\langle l'||\overleftarrow{\nabla}\cdot Y_L\overrightarrow{\nabla}||l\rangle
\end{aligned}
$$

Therefore one can get the result

$$
\begin{aligned}
\langle l'||\overleftarrow{\nabla}\cdot Y_L\overrightarrow{\nabla}||l\rangle &= (-)^{\frac{1}{2}(l+l')+L+l}\sum_{\eta=l\pm1}\sum_{\eta'=l'\pm1}\sqrt{\frac{(\eta'+l'+1)(\eta+l+1)(2L+1)(2\eta+1)(2\eta'+1)}{16\pi}} \\
&\times(-)^{\frac{1}{2}(\eta+\eta')}\begin{pmatrix} L & \eta' & \eta \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & l & L \\ \eta & \eta' & 1\end{Bmatrix} \\
&\times\left[\left(\frac{\overleftarrow{\partial}}{\partial r}+(-)^{\frac{1}{2}(\eta'-l'-1)}\frac{3l'-\eta'+1}{2r}\right)\right]\left[\left(\frac{\overrightarrow{\partial}}{\partial r}+(-)^{\frac{1}{2}(\eta-l-1)}\frac{3l-\eta+1}{2r}\right)\right]
\end{aligned}
$$

Using 3j,6j symbol's properties, one can get the relation

$$
\begin{aligned}
\begin{pmatrix} L & \eta' & \eta \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & l & L \\ \eta & \eta' & 1\end{Bmatrix} &= (-)^{1+l+l'}\Bigg[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} 1 & \eta' & l' \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} 1 & l & \eta \\ 0 & 0 & 0\end{pmatrix} \\
&\quad -\left(1+(-)^{L+\eta+\eta'}\right)\begin{pmatrix} L & l & l' \\ 0 & 1 & -1\end{pmatrix}\begin{pmatrix} 1 & \eta' & l' \\ -1 & 0 & 1\end{pmatrix}\begin{pmatrix} 1 & l & \eta \\ 1 & -1 & 0\end{pmatrix}\Bigg] \\
&= \frac{1}{2}\Bigg[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0\end{pmatrix}(-)^{\frac{1}{2}(\eta'-l'+\eta-l)}\sqrt{\frac{(\eta'+l'+1)(\eta+l+1)}{(2l'+1)(2\eta'+1)(2l+1)(2\eta+1)}} \\
&\quad +\left(1+(-)^{L+\eta+\eta'}\right)\begin{pmatrix} L & l & l' \\ 0 & 1 & -1\end{pmatrix}\sqrt{\frac{(3l'-\eta'+1)(3l-\eta+1)}{2(2l'+1)(2\eta'+1)(2l+1)(2\eta+1)}}\Bigg]
\end{aligned}
$$

Then

$$
\begin{aligned}
\langle l'||\overleftarrow{\nabla}\cdot Y_L\overrightarrow{\nabla}||l\rangle &= (-)^{L+l}\frac{1}{8}\sqrt{\frac{2L+1}{\pi(2l+1)(2l'+1)}}\sum_{\eta=l\pm1}\sum_{\eta'=l'\pm1} \\
&\times\Bigg[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0\end{pmatrix}(-)^{l'+l}(\eta'+l'+1)(\eta+l+1) \\
&+\left(1+(-)^{L+l+l'}\right)\begin{pmatrix} L & l & l' \\ 0 & 1 & -1\end{pmatrix}(-)^{\frac{1}{2}(\eta+l+\eta'+l')}\underline{\sqrt{\frac{(3l'-\eta'+1)(3l-\eta+1)(\eta'+l'+1)(\eta+l+1)}{2}}} \\
&\times\left[\left(\frac{\overleftarrow{\partial}}{\partial r}+(-)^{\frac{1}{2}(\eta'-l'-1)}\frac{3l'-\eta'+1}{2r}\right)\right]\left[\left(\frac{\overrightarrow{\partial}}{\partial r}+(-)^{\frac{1}{2}(\eta-l-1)}\frac{3l-\eta+1}{2r}\right)\right]
\end{aligned}
$$

For any $\eta(=l\pm1),\eta'(=l'\pm1)$, under line part of above becomes

$$
\sqrt{\frac{(3l'-\eta'+1)(3l-\eta+1)(\eta'+l'+1)(\eta+l+1)}{2}} = \sqrt{8l(l+1)l'(l'+1)}
$$

And by expanding summation above,

$$
\begin{aligned}
&\langle l'||\overleftarrow{\nabla}\cdot Y_L\overrightarrow{\nabla}||l\rangle \\
&= (-)^{L+l}\frac{1}{8}\sqrt{\frac{2L+1}{\pi(2l+1)(2l'+1)}}\sum_{\eta=l\pm1}\sum_{\eta'=l'\pm1} \\
&\times\Bigg[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}(-)^{l'+l}(\eta'+l'+1)(\eta+l+1) \\
&+\Big(1+(-)^{L+l+l'}\Big)\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}(-)^{\frac{1}{2}(\eta+l+\eta'+l')}\sqrt{8l(l+1)l'(l'+1)}\Bigg] \\
&\times\left[\left(\frac{\overleftarrow{\partial}}{\partial r}+(-)^{\frac{1}{2}(\eta'-l'-1)}\frac{3l'-\eta'+1}{2r}\right)\right]\left[\left(\frac{\overrightarrow{\partial}}{\partial r}+(-)^{\frac{1}{2}(\eta-l-1)}\frac{3l-\eta+1}{2r}\right)\right] \\
&= (-)^{l}\frac{1}{2}\sqrt{\frac{2L+1}{\pi(2l+1)(2l'+1)}} \\
&\Bigg\{\Bigg[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}(l'+1)(l+1)-\delta^{L+l+l'}_{=even}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}\sqrt{2l(l+1)l'(l'+1)}\Bigg]\left[\left(\frac{\overleftarrow{\partial}}{\partial r}+\frac{l'}{r}\right)\right]\left[\left(\frac{\overrightarrow{\partial}}{\partial r}+\frac{l}{r}\right)\right] \\
&+\Bigg[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}(l'+1)l+\delta^{L+l+l'}_{=even}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}\sqrt{2l(l+1)l'(l'+1)}\Bigg]\left[\left(\frac{\overleftarrow{\partial}}{\partial r}+\frac{l'}{r}\right)\right]\left[\left(\frac{\overrightarrow{\partial}}{\partial r}-\frac{l+1}{r}\right)\right] \\
&+\Bigg[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}l'(l+1)+\delta^{L+l+l'}_{=even}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}\sqrt{2l(l+1)l'(l'+1)}\Bigg]\left[\left(\frac{\overleftarrow{\partial}}{\partial r}-\frac{l'+1}{r}\right)\right]\left[\left(\frac{\overrightarrow{\partial}}{\partial r}+\frac{l}{r}\right)\right] \\
&+\Bigg[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}l'l-\delta^{L+l+l'}_{=even}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}\sqrt{2l(l+1)l'(l'+1)}\Bigg]\left[\left(\frac{\overleftarrow{\partial}}{\partial r}-\frac{l'+1}{r}\right)\right]\left[\left(\frac{\overrightarrow{\partial}}{\partial r}-\frac{l+1}{r}\right)\right]\Bigg\} \\
&= (-)^{l}\sqrt{\frac{2L+1}{4\pi(2l+1)(2l'+1)}} \\
&\Bigg\{\Bigg[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}(l'+1)(l+1)-\delta^{L+l+l'}_{=even}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}\sqrt{2l(l+1)l'(l'+1)}\Bigg]\left[\frac{\overleftarrow{\partial}}{\partial r}\frac{\overrightarrow{\partial}}{\partial r}+\frac{\overleftarrow{\partial}}{\partial r}\frac{l}{r}+\frac{l'}{r}\frac{\overrightarrow{\partial}}{\partial r}+\frac{l'l}{r^2}\right] \\
&+\Bigg[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}(l'+1)l+\delta^{L+l+l'}_{=even}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}\sqrt{2l(l+1)l'(l'+1)}\Bigg]\left[\frac{\overleftarrow{\partial}}{\partial r}\frac{\overrightarrow{\partial}}{\partial r}-\frac{\overleftarrow{\partial}}{\partial r}\frac{l+1}{r}+\frac{l'}{r}\frac{\overrightarrow{\partial}}{\partial r}-\frac{l'}{r}\frac{l+1}{r}\right] \\
&+\Bigg[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}l'(l+1)+\delta^{L+l+l'}_{=even}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}\sqrt{2l(l+1)l'(l'+1)}\Bigg]\left[\frac{\overleftarrow{\partial}}{\partial r}\frac{\overrightarrow{\partial}}{\partial r}+\frac{\overleftarrow{\partial}}{\partial r}\frac{l}{r}-\frac{l'+1}{r}\frac{\overrightarrow{\partial}}{\partial r}-\frac{l(l'+1)}{r^2}\right] \\
&+\Bigg[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}l'l-\delta^{L+l+l'}_{=even}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}\sqrt{2l(l+1)l'(l'+1)}\Bigg]\left[\frac{\overleftarrow{\partial}}{\partial r}\frac{\overrightarrow{\partial}}{\partial r}-\frac{\overleftarrow{\partial}}{\partial r}\frac{l+1}{r}-\frac{l'+1}{r}\frac{\overrightarrow{\partial}}{\partial r}+\frac{(l+1)(l'+1)}{r^2}\right] \\
&= (-)^{l}\sqrt{\frac{(2L+1)(2l'+1)(2l+1)}{4\pi}}\left[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}\frac{\overleftarrow{\partial}}{\partial r}\frac{\overrightarrow{\partial}}{\partial r}-\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}\frac{\sqrt{2l(l+1)l'(l'+1)}}{r^2}\right]
\end{aligned}
$$

Thus finally, one could get the result

$$
\langle l'||\overleftarrow{\nabla}\cdot Y_L\overrightarrow{\nabla}||l\rangle = (-)^{l}\sqrt{\frac{(2L+1)(2l'+1)(2l+1)}{4\pi}}\left[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}\frac{\overleftarrow{\partial}}{\partial r}\frac{\overrightarrow{\partial}}{\partial r}-\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}\frac{\sqrt{2l(l+1)l'(l'+1)}}{r^2}\right]
$$

Appendix D

3j and 6j symbol

D.1 Clebsch-Gordan coefficient and 3j-symbol

The definition of the relation between clebsch-gordan coefficient and 3j-symbol is given by

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \frac{(-)^{j_1-j_2-m_3}}{\sqrt{2j_3+1}} \langle j_1 m_1 : j_2 m_2 | j_3 - m_3 \rangle$$

D.1.1 Symmetry property

Clebsch-Gordan's coefficients have important properties

$$\langle j_1 m_1 : j_2 m_2 | j_3 m_3 \rangle = (-)^{j_1+j_2-j_3} \langle j_1 - m_1 : j_2 - m_2 | j_3 - m_3 \rangle$$

and

$$\begin{aligned} \langle j_1 m_1 : j_2 m_2 | j_3 m_3 \rangle &= (-)^{j_1+j_2-j_3} \langle j_2 m_2 : j_1 m_1 | j_3 m_3 \rangle \\ &= (-)^{j_1-m_1} \left(\frac{2j_3+1}{2j_2+1} \right)^{1/2} \langle j_1 m_1 : j_3 - m_3 | j_2 - m_2 \rangle \\ &= (-)^{j_2+m_2} \left(\frac{2j_3+1}{2j_1+1} \right)^{1/2} \langle j_3 - m_3 : j_2 m_2 | j_1 - m_1 \rangle \end{aligned}$$

These properties can be expressed by 3j-symbol's language

$$\begin{aligned} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= (-)^{j_1+j_2-j_3-2m_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} \\ &= (-)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} \end{aligned}$$

Note that when j_3 is integer, m_3 is also integer. Then $(-)^{-j_3} = (-)^{j_3}$ and $(-)^{2m_3} = 1$. And also when j_3 is half-integer, m_3 is also half-integer. Then $(-)^{-2m_3} = -1$ and $(-)^{-j_3-1} = (-)^{j_3}$. So in both case, j_3 is integer or half-integer,

$$(-)^{j_1+j_2-j_3-2m_3} = (-)^{j_1+j_2+j_3}$$

Also 2nd properties of CG coef. can be expressed as

$$\begin{aligned} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= (-)^{-j_1-j_2-j_3} \begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix} \\ &= (-)^{-j_1-j_2-j_3} \begin{pmatrix} j_1 & j_3 & j_2 \\ m_1 & m_3 & m_2 \end{pmatrix} \\ &= (-)^{-j_1-j_2-j_3} \begin{pmatrix} j_3 & j_2 & j_1 \\ m_3 & m_2 & m_1 \end{pmatrix} \end{aligned}$$

In addition, the desired recursion relation for the C.G. coef.

$$\sqrt{(j_3 \mp m_3)(j_3 \pm m_3 + 1)}\langle j_1 m_1 : j_2 m_2 | j_3 m_3 \pm 1\rangle$$
$$= \sqrt{(j_1 \mp m_1 + 1)(j_1 \pm m_1)}\langle j_1 m_1 \mp 1 : j_2 m_2 | j_3 m_3\rangle + \sqrt{(j_2 \mp m_2 + 1)(j_2 \pm m_2)}\langle j_1 m_1 : j_2 m_2 \mp 1 | j_3 m_3\rangle$$

In the 3j-symbol's language, this relation can be expressed as

$$\sqrt{(j_3 \mp m_3 + 1)(j_3 \pm m_3)} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \mp 1 \end{pmatrix}$$
$$= \sqrt{(j_1 \mp m_1 + 1)(j_1 \pm m_1)} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 \mp 1 & m_2 & m_3 \end{pmatrix} + \sqrt{(j_2 \mp m_2 + 1)(j_2 \pm m_2)} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 \mp 1 & m_3 \end{pmatrix}$$

If one puts $j_1 = l', m_1 = 0, j_2 = l, m_2 = 0, j_3 = L, m_3 = -1$, and takes lower sign, then one can get

$$\sqrt{L(L+1)} \begin{pmatrix} l' & l & L \\ 0 & 0 & 0 \end{pmatrix} = \sqrt{l'(l'+1)} \begin{pmatrix} l' & l & L \\ 1 & 0 & -1 \end{pmatrix} + \sqrt{l(l+1)} \begin{pmatrix} l' & l & L \\ 0 & 1 & -1 \end{pmatrix}$$

D.2 Racah coefficient and 6j-symbol

Racah coefficient and 6j-symbol can be related as

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = (-)^{j_1+j_2+l_1+l_2} W(j_1, j_2, l_2, l_1; j_3, l_2) \qquad \textit{Edmonds p97 (6.2.13)}$$

memo....

$$[6l(l+1)(2l+1)]^{1/2} \langle l0 : 10|\eta 0\rangle W(l\eta 11 : 1l)$$
$$= (-)^{l+1} [6l(l+1)(2l+1)]^{1/2} \sqrt{2\eta+1} \begin{pmatrix} l & 1 & \eta \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l & \eta & 1 \\ 1 & 1 & l \end{Bmatrix}$$
$$= (-)^{l+1} [6l(l+1)(2l+1)]^{1/2} \sqrt{2\eta+1} \begin{pmatrix} l & 1 & \eta \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l & 1 & \eta \\ 1 & l & 1 \end{Bmatrix}$$
$$= [6l(l+1)(2l+1)]^{1/2} \sqrt{2\eta+1} \sum_{m_1=-1,0,+1}$$
$$\times \begin{pmatrix} l & l & 1 \\ 0 & m_1 & -m_1 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ -m_1 & 0 & m_1 \end{pmatrix} \begin{pmatrix} 1 & l & \eta \\ m_1 & -m_1 & 0 \end{pmatrix}$$
$$= [6l(l+1)(2l+1)]^{1/2} \sqrt{2\eta+1}$$
$$\times \Big\{ 2 \begin{pmatrix} l & l & 1 \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & l & \eta \\ 1 & -1 & 0 \end{pmatrix}$$
$$+ \begin{pmatrix} l & l & 1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l & \eta \\ 0 & 0 & 0 \end{pmatrix} \Big\}$$
$$= (-)^{l+1} \sqrt{2l(l+1)(2\eta+1)} \begin{pmatrix} 1 & l & \eta \\ 1 & -1 & 0 \end{pmatrix}$$
$$= -\sqrt{\frac{l(l+1)(3l-\eta+1)}{2(2l+1)}} = \begin{cases} (\eta = l+1) & -l\sqrt{\frac{l+1}{2l+1}} \\ (\eta = l-1) & -(l+1)\sqrt{\frac{l}{2l+1}} \end{cases}$$

Appendix E

Useful formulas

E.1 Reduced matrix element $\langle l'||Y_L||l\rangle$

$$\begin{aligned}
\langle l'm'|Y_{LM}|lm\rangle &= \int d\hat{\boldsymbol{r}} Y^*_{l'm'}(\hat{\boldsymbol{r}})Y_{LM}(\hat{\boldsymbol{r}})Y_{lm}(\hat{\boldsymbol{r}}) \\
&= \sqrt{\frac{(2L+1)(2l+1)}{4\pi(2l'+1)}}\langle L0:l0|l'0\rangle\langle LM:lm|l'm'\rangle \\
&= (-)^{m'}\sqrt{\frac{(2L+1)(2l+1)(2l'+1)}{4\pi}}\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} L & l & l' \\ M & m & -m' \end{pmatrix} \\
&= (-)^{m'}\sqrt{\frac{(2L+1)(2l+1)(2l'+1)}{4\pi}}\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l' & L & l \\ -m' & M & m \end{pmatrix}
\end{aligned}$$

Wigner-Eckart's theorem is given by

$$\langle l'm'|Y_{LM}|lm\rangle = (-)^{l'-m'}\begin{pmatrix} l' & L & l \\ -m' & M & m \end{pmatrix}\langle l'||Y_L||l\rangle$$

Threfore

$$\langle l'||Y_L||l\rangle = (-)^{l'}\sqrt{\frac{(2L+1)(2l+1)(2l'+1)}{4\pi}}\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}$$

E.2 Reduced matrix element including the spherical harmonics

Next one calculates this value

$$\int d\hat{\boldsymbol{r}}\boldsymbol{Y}^*_{l'\eta'm'_l}(\hat{\boldsymbol{r}})\cdot Y_{LM}(\hat{\boldsymbol{r}})\boldsymbol{Y}_{l\eta m_l}(\hat{\boldsymbol{r}})$$

Here the vector-spherical harmonics is defined as

$$\begin{aligned}
\boldsymbol{Y}_{l\eta m_l}(\hat{\boldsymbol{r}}) &= \sum_{m_\eta,q}\langle\eta m_\eta:1q|lm_l\rangle Y_{\eta m_\eta}(\hat{\boldsymbol{r}})\boldsymbol{e}_q \\
&= (-)^{1-\eta-m_l}\sum_{m_\eta,q}\begin{pmatrix} \eta & 1 & l \\ m_\eta & q & -m_l \end{pmatrix}Y_{\eta m_\eta}(\hat{\boldsymbol{r}})\boldsymbol{e}_q
\end{aligned}$$

Therefore

$$
\begin{aligned}
&\int d\hat{\boldsymbol{r}} \boldsymbol{Y}^*_{l'\eta' m_l'}(\hat{\boldsymbol{r}}) \cdot Y_{LM}(\hat{\boldsymbol{r}}) \boldsymbol{Y}_{l\eta m_l}(\hat{\boldsymbol{r}}) \\
&= \sqrt{(2l+1)(2l'+1)}(-)^{l+m_l+l'+m_{l'}} \\
&\qquad \times \sum_{m_{\eta'}} \sum_{m_\eta} \sum_q \begin{pmatrix} \eta' & 1 & l' \\ m_{\eta'} & q & -m_{l'} \end{pmatrix} \begin{pmatrix} \eta & 1 & l \\ m_\eta & q & -m_l \end{pmatrix} \int d\hat{\boldsymbol{r}} Y^*_{\eta' m_{\eta'}}(\hat{\boldsymbol{r}}) Y_{LM}(\hat{\boldsymbol{r}}) Y_{\eta m_\eta}(\hat{\boldsymbol{r}}) \\
&= \sqrt{(2l+1)(2l'+1)}(-)^{l+m_l+l'+m_{l'}} \\
&\qquad \times \sum_{m_{\eta'}} \sum_{m_\eta} \sum_q (-)^{\eta'+m_{\eta'}} \begin{pmatrix} \eta' & 1 & l' \\ m_{\eta'} & q & -m_{l'} \end{pmatrix} \begin{pmatrix} \eta & 1 & l \\ m_\eta & q & -m_l \end{pmatrix} \begin{pmatrix} \eta' & L & \eta \\ -m_{\eta'} & M & m_\eta \end{pmatrix} \langle \eta' || Y_L || \eta \rangle \\
&= \sqrt{(2l+1)(2l'+1)}(-)^{l+m_l+l'+m_{l'}} (-)^{L+l+l'} (-)^{-\eta-1} \\
&\times \sum_{m_{\eta'}} \sum_{m_\eta} \sum_q (-)^{m_\eta - q} (-)^{\eta+\eta'+1+q-m_\eta-m_{\eta'}} \begin{pmatrix} l' & 1 & \eta' \\ -m_{l'} & q & m_{\eta'} \end{pmatrix} \begin{pmatrix} \eta & L & \eta' \\ m_\eta & M & -m_{\eta'} \end{pmatrix} \begin{pmatrix} \eta & 1 & l \\ -m_\eta & -q & m_l \end{pmatrix} \langle \eta' || Y_L || \eta \rangle \\
&(-)^{m_\eta - q} = (-)^{-m_\eta - q} = (-)^{m_l} \qquad \text{(3j-symbol's property)} \\
&= \sqrt{(2l+1)(2l'+1)}(-)^{l'+m_{l'}} (-)^{L+l+l'} \\
&\times \sum_{m_{\eta'}} \sum_{m_\eta} \sum_q (-)^{\eta+\eta'+1+q-m_\eta-m_{\eta'}} \begin{pmatrix} l' & 1 & \eta' \\ -m_{l'} & q & m_{\eta'} \end{pmatrix} \begin{pmatrix} \eta & L & \eta' \\ m_\eta & M & -m_{\eta'} \end{pmatrix} \begin{pmatrix} \eta & 1 & l \\ -m_\eta & -q & m_l \end{pmatrix} \langle \eta' || Y_L || \eta \rangle \\
&= \sqrt{(2l+1)(2l'+1)}(-)^{l'+m_{l'}} (-)^{L+l+l'} \begin{pmatrix} l' & L & l \\ -m_{l'} & M & m_l \end{pmatrix} \begin{Bmatrix} l' & L & l \\ \eta & 1 & \eta' \end{Bmatrix} \langle \eta' || Y_L || \eta \rangle \\
&= \sqrt{\frac{(2l+1)(2l'+1)(2\eta+1)(2\eta'+1)}{4\pi}} (-)^{m_{l'}+1} \begin{pmatrix} l' & L & l \\ -m_{l'} & M & m_l \end{pmatrix} \begin{Bmatrix} l' & L & l \\ \eta & 1 & \eta' \end{Bmatrix} \begin{pmatrix} L & \eta & \eta' \\ 0 & 0 & 0 \end{pmatrix}
\end{aligned}
$$

E.3 $\langle l'm' | \boldsymbol{Y}_{L\lambda M} \cdot \hat{\boldsymbol{r}} | lm \rangle$

E.3.1 The simplest way

$$
\begin{aligned}
& \hat{\boldsymbol{r}} \cdot \boldsymbol{Y}_{L\lambda M} \\
= & \sum_{m_\lambda, q} \langle \lambda m_\lambda : 1q | LM \rangle \hat{\boldsymbol{r}} Y_{\lambda m_\lambda} \cdot \boldsymbol{e}_q \\
= & \sum_{m_\lambda, q} \langle \lambda m_\lambda : 1q | LM \rangle \left\{ -\left(\frac{\lambda+1}{2\lambda+1} \right)^{\frac{1}{2}} \boldsymbol{Y}_{\lambda \lambda+1 m_\lambda} + \left(\frac{\lambda}{2\lambda+1} \right)^{\frac{1}{2}} \boldsymbol{Y}_{\lambda \lambda-1 m_\lambda} \right\} \cdot \boldsymbol{e}_q \\
= & \sum_{m_\lambda, q} \langle \lambda m_\lambda : 1q | LM \rangle (-)^q \\
& \times \left\{ -\left(\frac{\lambda+1}{2\lambda+1} \right)^{\frac{1}{2}} \sum_{m'_\lambda} \langle \lambda+1, m'_\lambda : 1-q | \lambda m_\lambda \rangle Y_{\lambda+1, m'_\lambda} + \left(\frac{\lambda}{2\lambda+1} \right)^{\frac{1}{2}} \sum_{m'_\lambda} \langle \lambda-1, m'_\lambda : 1-q | \lambda m_\lambda \rangle Y_{\lambda-1, m'_\lambda} \right\} \\
= & \sum_{m_\lambda, q} \langle \lambda m_\lambda : 1q | LM \rangle \\
& \times \left\{ \left(\frac{\lambda+1}{2\lambda+3} \right)^{\frac{1}{2}} \sum_{m'_\lambda} \langle \lambda, -m_\lambda : 1-q | \lambda+1, m'_\lambda \rangle Y_{\lambda+1, m'_\lambda} - \left(\frac{\lambda}{2\lambda-1} \right)^{\frac{1}{2}} \sum_{m'_\lambda} \langle \lambda, -m_\lambda : 1-q | \lambda-1, m'_\lambda \rangle Y_{\lambda-1, m'_\lambda} \right\} \\
= & \sum_{m'_\lambda} \left(\left(\frac{\lambda+1}{2\lambda+3} \right)^{\frac{1}{2}} \delta_{\lambda=L-1} \delta_{m'_\lambda=M} Y_{\lambda+1, m'_\lambda} - \left(\frac{\lambda}{2\lambda-1} \right)^{\frac{1}{2}} \delta_{\lambda=L+1} \delta_{m'_\lambda=M} Y_{\lambda-1, m'_\lambda} \right) \\
= & \left[\left(\frac{L}{2L+1} \right)^{\frac{1}{2}} \delta_{\lambda=L-1} - \left(\frac{L+1}{2L+1} \right)^{\frac{1}{2}} \delta_{\lambda=L+1} \right] Y_{LM}
\end{aligned}
$$

Therefore one can get

$$\begin{aligned}
\langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot\hat{\boldsymbol{r}}|lm\rangle &= \int d\hat{\boldsymbol{r}} Y^*_{l'm'}\boldsymbol{Y}_{L\lambda M}\cdot\hat{\boldsymbol{r}} Y_{lm} \\
&= \left[\int d\hat{\boldsymbol{r}} Y^*_{lm}\hat{\boldsymbol{r}}\cdot\boldsymbol{Y}^*_{L\lambda M} Y_{l'm'}\right]^* \\
&= \left[\left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\delta_{\lambda=L-1} - \left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\delta_{\lambda=L+1}\right]\langle l'm'|Y_{LM}|lm\rangle
\end{aligned}$$

E.3.2 Somewhat complicated way

On the other hand, one can calculate by another way. This way is rather complicated, but one can prove this way is equivalent with the previous way as follows.

$$\begin{aligned}
&\langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot\hat{\boldsymbol{r}}|lm\rangle \\
= &\int d\hat{\boldsymbol{r}} Y^*_{l'm'}\boldsymbol{Y}_{L\lambda M}\cdot\underline{\hat{\boldsymbol{r}} Y_{lm}} \\
= &\int d\hat{\boldsymbol{r}} Y^*_{l'm'}\boldsymbol{Y}_{L\lambda M}\cdot\left\{-\left(\frac{l+1}{2l+1}\right)^{\frac{1}{2}}\boldsymbol{Y}_{ll+1m} + \left(\frac{l}{2l+1}\right)^{\frac{1}{2}}\boldsymbol{Y}_{ll-1m}\right\} \\
= &(-)^{m+M}\left[\frac{(2l+1)(2l'+1)(2L+1)(2\lambda+1)}{4\pi}\right]^{\frac{1}{2}}\begin{pmatrix} l' & L & l \\ -m' & M & m\end{pmatrix} \\
&\times\left[\left[\frac{(l+1)(2l+3)}{2l+1}\right]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l+1 \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & \lambda & l+1 \\ 1 & l & L\end{Bmatrix} - \left[\frac{l(2l-1)}{2l+1}\right]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l-1 \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & \lambda & l-1 \\ 1 & l & L\end{Bmatrix}\right] \\
= &\langle l'm'|Y_{LM}|lm\rangle\frac{1}{\begin{pmatrix} l' & L & l \\ 0 & 0 & 0\end{pmatrix}} \\
&\times\left[\left[\frac{(l+1)(2l+3)(2\lambda+1)}{2l+1}\right]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l+1 \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & \lambda & l+1 \\ 1 & l & L\end{Bmatrix}\right. \\
&\qquad\left. - \left[\frac{l(2l-1)(2\lambda+1)}{2l+1}\right]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l-1 \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & \lambda & l-1 \\ 1 & l & L\end{Bmatrix}\right] \\
= &(-)^{\frac{1}{2}(\lambda+3L+1)}\left[\frac{(\lambda+L+1)}{2(2L+1)}\right]^{\frac{1}{2}}\langle l'm'|Y_{LM}|lm\rangle = \left[\left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\delta_{\lambda=L-1} - \left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\delta_{\lambda=L+1}\right]\langle l'm'|Y_{LM}|lm\rangle
\end{aligned}$$

where

$$\begin{aligned}
&\left[\frac{(l+1)(2l+3)(2\lambda+1)}{2l+1}\right]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l+1 \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & \lambda & l+1 \\ 1 & l & L\end{Bmatrix} \\
&\quad = \frac{1+(-)^{L+l+l'}}{2}\frac{1}{2l+1}\left[\frac{l(l+1)(3L-\lambda+1)}{2(2L+1)}\right]^{\frac{1}{2}}\begin{pmatrix} l' & l & L \\ 0 & 1 & -1\end{pmatrix} \\
&\qquad\qquad + (-)^{\frac{1}{2}(\lambda+3L+1)}\frac{l+1}{2l+1}\left[\frac{(\lambda+L+1)}{2(2L+1)}\right]^{\frac{1}{2}}\begin{pmatrix} l' & l & L \\ 0 & 0 & 0\end{pmatrix}
\end{aligned}$$

$$\begin{aligned}
&\left[\frac{l(2l-1)(2\lambda+1)}{2l+1}\right]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l-1 \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & \lambda & l-1 \\ 1 & l & L\end{Bmatrix} \\
&\quad = \frac{1+(-)^{L+l+l'}}{2}\frac{1}{2l+1}\left[\frac{l(l+1)(3L-\lambda+1)}{2(2L+1)}\right]^{\frac{1}{2}}\begin{pmatrix} l' & l & L \\ 0 & 1 & -1\end{pmatrix} \\
&\qquad\qquad - (-)^{\frac{1}{2}(\lambda+3L+1)}\frac{l}{2l+1}\left[\frac{(\lambda+L+1)}{2(2L+1)}\right]^{\frac{1}{2}}\begin{pmatrix} l' & l & L \\ 0 & 0 & 0\end{pmatrix}
\end{aligned}$$

E.4 $\langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\boldsymbol{L}|lm\rangle$

$$\begin{aligned}
&\langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\boldsymbol{L}|lm\rangle\\
=\;& \int d\hat{\boldsymbol{r}} Y^*_{l'm'}\boldsymbol{Y}_{L\lambda M}\cdot \underline{i\boldsymbol{r}\hat{\times}\boldsymbol{L}Y_{lm}}\\
=\;& \int d\hat{\boldsymbol{r}} Y^*_{l'm'}\boldsymbol{Y}_{L\lambda M}\cdot\left\{-l\left(\frac{l+1}{2l+1}\right)^{\frac{1}{2}}\boldsymbol{Y}_{ll+1m}-(l+1)\left(\frac{l}{2l+1}\right)^{\frac{1}{2}}\boldsymbol{Y}_{ll-1m}\right\}\\
=\;& (-)^{m+M}\left[\frac{(2l+1)(2l'+1)(2L+1)(2\lambda+1)}{4\pi}\right]^{\frac{1}{2}}\begin{pmatrix} l' & L & l\\ -m' & M & m\end{pmatrix}\\
&\times\Bigg[l\left[\frac{(l+1)(2l+3)}{2l+1}\right]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l+1\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & \lambda & l+1\\ 1 & l & L\end{Bmatrix}\\
&\qquad +(l+1)\left[\frac{l(2l-1)}{2l+1}\right]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l-1\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & \lambda & l-1\\ 1 & l & L\end{Bmatrix}\Bigg]\\
=\;& \langle l'm'|Y_{LM}|lm\rangle\frac{1}{\begin{pmatrix} l' & L & l\\ 0 & 0 & 0\end{pmatrix}}\\
&\times\Bigg[l\left[\frac{(l+1)(2l+3)(2\lambda+1)}{2l+1}\right]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l+1\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & \lambda & l+1\\ 1 & l & L\end{Bmatrix}\\
&\qquad +(l+1)\left[\frac{l(2l-1)(2\lambda+1)}{2l+1}\right]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l-1\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & \lambda & l-1\\ 1 & l & L\end{Bmatrix}\Bigg]\\
=\;& \frac{1+(-)^{L+l+l'}}{2}\left[\frac{3L-\lambda+1}{2(2L+1)}\right]^{\frac{1}{2}}\frac{\sqrt{l(l+1)}\begin{pmatrix} l' & l & L\\ 0 & 1 & -1\end{pmatrix}}{\begin{pmatrix} l' & L & l\\ 0 & 0 & 0\end{pmatrix}}\langle l'm'|Y_{LM}|lm\rangle
\end{aligned}$$

where

$$\begin{aligned}
&l\left[\frac{(l+1)(2l+3)(2\lambda+1)}{2l+1}\right]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l+1\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & \lambda & l+1\\ 1 & l & L\end{Bmatrix}\\
&\quad=\frac{1+(-)^{L+l+l'}}{2}\frac{l}{2l+1}\left[\frac{l(l+1)(3L-\lambda+1)}{2(2L+1)}\right]^{\frac{1}{2}}\begin{pmatrix} l' & l & L\\ 0 & 1 & -1\end{pmatrix}\\
&\qquad +(-)^{\frac{1}{2}(\lambda+3L+1)}\frac{l(l+1)}{2l+1}\left[\frac{(\lambda+L+1)}{2(2L+1)}\right]^{\frac{1}{2}}\begin{pmatrix} l' & l & L\\ 0 & 0 & 0\end{pmatrix}
\end{aligned}$$

$$\begin{aligned}
&(l+1)\left[\frac{l(2l-1)(2\lambda+1)}{2l+1}\right]^{\frac{1}{2}}\begin{pmatrix} l' & \lambda & l-1\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & \lambda & l-1\\ 1 & l & L\end{Bmatrix}\\
&\quad=\frac{1+(-)^{L+l+l'}}{2}\frac{l+1}{2l+1}\left[\frac{l(l+1)(3L-\lambda+1)}{2(2L+1)}\right]^{\frac{1}{2}}\begin{pmatrix} l' & l & L\\ 0 & 1 & -1\end{pmatrix}\\
&\qquad -(-)^{\frac{1}{2}(\lambda+3L+1)}\frac{l(l+1)}{2l+1}\left[\frac{(\lambda+L+1)}{2(2L+1)}\right]^{\frac{1}{2}}\begin{pmatrix} l' & l & L\\ 0 & 0 & 0\end{pmatrix}
\end{aligned}$$

Next one thinks the inverce term

$$\begin{aligned}
\langle l'm'|i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot\boldsymbol{Y}_{L\lambda M}|lm\rangle &= \langle lm|\boldsymbol{Y}^*_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}|l'm'\rangle^* \\
&= (-)^M\langle lm|\boldsymbol{Y}_{L\lambda -M}\cdot i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}|l'm'\rangle^* \\
&= (-)^M\frac{1+(-)^{L+l+l'}}{2}\left[\frac{3L-\lambda+1}{2(2L+1)}\right]^{\frac{1}{2}}\frac{\sqrt{l'(l'+1)}\begin{pmatrix} l & l' & L \\ 0 & 1 & -1\end{pmatrix}}{\begin{pmatrix} l' & L & l \\ 0 & 0 & 0\end{pmatrix}}\langle lm|Y_{L-M}|l'm'\rangle^* \\
&= \frac{1+(-)^{L+l+l'}}{2}\left[\frac{3L-\lambda+1}{2(2L+1)}\right]^{\frac{1}{2}}\frac{\sqrt{l'(l'+1)}\begin{pmatrix} l & l' & L \\ 0 & 1 & -1\end{pmatrix}}{\begin{pmatrix} l' & L & l \\ 0 & 0 & 0\end{pmatrix}}\langle l'm'|Y_{LM}|lm\rangle \\
&= \frac{1+(-)^{L+l+l'}}{2}\left[\frac{3L-\lambda+1}{2(2L+1)}\right]^{\frac{1}{2}}\frac{1}{\begin{pmatrix} l' & L & l \\ 0 & 0 & 0\end{pmatrix}} \\
&\quad\times\left[-\sqrt{L(L+1)}\begin{pmatrix} l & l' & L \\ 0 & 0 & 0\end{pmatrix}-\sqrt{l(l+1)}\begin{pmatrix} l' & l & L \\ 0 & 1 & -1\end{pmatrix}\right]\langle l'm'|Y_{LM}|lm\rangle \\
&= -\frac{1+(-)^{L+l+l'}}{2}\left[\frac{L(L+1)(3L-\lambda+1)}{2(2L+1)}\right]^{\frac{1}{2}}\langle l'm'|Y_{LM}|lm\rangle-\langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\boldsymbol{L}|lm\rangle
\end{aligned}$$

Therefore

$$\langle l'm'|i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot\boldsymbol{Y}_{L\lambda M}+\boldsymbol{Y}_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}|lm\rangle = -\frac{1+(-)^{L+l+l'}}{2}\left[\frac{L(L+1)(3L-\lambda+1)}{2(2L+1)}\right]^{\frac{1}{2}}\langle l'm'|Y_{LM}|lm\rangle$$

$$\begin{aligned}
&\langle l'm'|i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot\boldsymbol{Y}_{L\lambda M}-\boldsymbol{Y}_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}|lm\rangle \\
&\quad= -\frac{1+(-)^{L+l+l'}}{2}\left[\frac{L(L+1)(3L-\lambda+1)}{2(2L+1)}\right]^{\frac{1}{2}}\langle l'm'|Y_{LM}|lm\rangle-2\langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\boldsymbol{L}|lm\rangle
\end{aligned}$$

$$\begin{aligned}
\langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\boldsymbol{L}|lm\rangle &= \frac{1+(-)^{L+l+l'}}{2}\left[\frac{3L-\lambda+1}{2(2L+1)}\right]^{\frac{1}{2}}\frac{\sqrt{l(l+1)}\begin{pmatrix} l' & l & L \\ 0 & 1 & -1\end{pmatrix}}{\begin{pmatrix} l' & L & l \\ 0 & 0 & 0\end{pmatrix}}\langle l'm'|Y_{LM}|lm\rangle \\
&= -\frac{1+(-)^{L+l+l'}}{2}\left[\frac{3L-\lambda+1}{2(2L+1)}\right]^{\frac{1}{2}}\sqrt{l(l+1)}\frac{\langle l1:l'0|L1\rangle}{\langle l0:l'0|L0\rangle}\langle l'm'|Y_{LM}|lm\rangle
\end{aligned}$$

E.5 The derivation of $\langle l'm'|\nabla\cdot Y_{LM}\nabla|lm\rangle$

$$
\begin{aligned}
&\langle l'm'|\hat{\boldsymbol{r}}\cdot Y_{LM}\hat{\boldsymbol{r}}|lm\rangle \\
&=\int d\hat{\boldsymbol{r}}\left(-\left[\frac{l'+1}{2l'+1}\right]^{\frac{1}{2}}\boldsymbol{Y}^*_{l'l'+1m'}+\left[\frac{l'}{2l'+1}\right]^{\frac{1}{2}}\boldsymbol{Y}^*_{l'l'-1m'}\right) \\
&\qquad\cdot Y_{LM}\left(-\left[\frac{l+1}{2l+1}\right]^{\frac{1}{2}}\boldsymbol{Y}_{ll+1m}+\left[\frac{l}{2l+1}\right]^{\frac{1}{2}}\boldsymbol{Y}_{ll-1m}\right) \\
&=\sum_{\eta=l\pm1}\sum_{\eta'=l'\pm1}(-)^{\frac{1}{2}(\eta-l+\eta'-l')+1}\left[\frac{(\eta'+l'+1)(\eta+l+1)}{2(2l'+1)2(2l+1)}\right]^{\frac{1}{2}}\int d\hat{\boldsymbol{r}}\boldsymbol{Y}^*_{l'\eta'm'}Y_{LM}\boldsymbol{Y}_{l\eta m} \\
&=\frac{(-)^{m'+1}}{2}\left[\frac{2L+1}{4\pi}\right]^{\frac{1}{2}}\begin{pmatrix} l' & L & l \\ -m' & M & m\end{pmatrix} \\
&\times\sum_{\eta=l\pm1}\sum_{\eta'=l'\pm1}\left[-\begin{pmatrix} L & l & l' \\ 0 & 0 & 0\end{pmatrix}\frac{(\eta'+l'+1)(\eta+l+1)}{[2(2l'+1)2(2l+1)]^{\frac{1}{2}}}\right. \\
&\qquad\left.+(-)^{\frac{1}{2}(\eta-l+\eta'-l')+1}\frac{1+(-)^{L+l+l'}}{2}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1\end{pmatrix}\left[\frac{4l'(l'+1)4l(l+1)}{2(2l'+1)2(2l+1)}\right]^{\frac{1}{2}}\right] \\
&=(-)^{m'}\left[\frac{(2L+1)(2l'+1)(2l+1)}{4\pi}\right]^{\frac{1}{2}}\begin{pmatrix} l' & L & l \\ -m' & M & m\end{pmatrix}\begin{pmatrix} L & l & l' \\ 0 & 0 & 0\end{pmatrix}=\langle l'm'|Y_{LM}|lm\rangle
\end{aligned}
$$

$$
\begin{aligned}
&\langle l'm'|\hat{\boldsymbol{r}}\cdot Y_{LM}i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}|lm\rangle \\
&=\int d\hat{\boldsymbol{r}}\left(-\left[\frac{l'+1}{2l'+1}\right]^{\frac{1}{2}}\boldsymbol{Y}^*_{l'l'+1m'}+\left[\frac{l'}{2l'+1}\right]^{\frac{1}{2}}\boldsymbol{Y}^*_{l'l'-1m'}\right) \\
&\qquad\cdot Y_{LM}\left(-l\left[\frac{l+1}{2l+1}\right]^{\frac{1}{2}}\boldsymbol{Y}_{ll+1m}-(l+1)\left[\frac{l}{2l+1}\right]^{\frac{1}{2}}\boldsymbol{Y}_{ll-1m}\right) \\
&=\sum_{\eta=l\pm1}\sum_{\eta'=l'\pm1}(-)^{\frac{1}{2}(\eta'-l'+1)}\frac{\sqrt{(3l-\eta+1)(\eta'+l'+1)}}{2}\left[\frac{l(l+1)}{(2l'+1)(2l+1)}\right]^{\frac{1}{2}}\int d\hat{\boldsymbol{r}}\boldsymbol{Y}^*_{l'\eta'm'}Y_{LM}\boldsymbol{Y}_{l\eta m} \\
&=0
\end{aligned}
$$

$$
\begin{aligned}
&\langle l'm'|i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot Y_{LM}i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}|lm\rangle \\
&=\int d\hat{\boldsymbol{r}}\left(l'\left[\frac{l'+1}{2l'+1}\right]^{\frac{1}{2}}\boldsymbol{Y}^*_{l'l'+1m'}+(l'+1)\left[\frac{l'}{2l'+1}\right]^{\frac{1}{2}}\boldsymbol{Y}^*_{l'l'-1m'}\right) \\
&\qquad\cdot Y_{LM}\left(l\left[\frac{l+1}{2l+1}\right]^{\frac{1}{2}}\boldsymbol{Y}_{ll+1m}+(l+1)\left[\frac{l}{2l+1}\right]^{\frac{1}{2}}\boldsymbol{Y}_{ll-1m}\right) \\
&=\sum_{\eta=l\pm1}\sum_{\eta'=l'\pm1}\frac{(3l'-\eta'+1)(3\eta-l+1)}{4}\left[\frac{(\eta'+l'+1)(\eta+l+1)}{2(2l'+1)2(2l+1)}\right]^{\frac{1}{2}}\int d\hat{\boldsymbol{r}}\boldsymbol{Y}^*_{l'\eta'm'}Y_{LM}\boldsymbol{Y}_{l\eta m} \\
&=\frac{(-)^{m'+1}}{2}\left[\frac{2L+1}{4\pi}\right]^{\frac{1}{2}}\begin{pmatrix} l' & L & l \\ -m' & M & m\end{pmatrix}\left[\frac{l(l+1)l'(l'+1)}{(2l'+1)(2l+1)}\right]^{\frac{1}{2}} \\
&\times\sum_{\eta=l\pm1}\sum_{\eta'=l'\pm1}\left[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0\end{pmatrix}(-)^{\frac{1}{2}(\eta'-l'+\eta-l)}2\sqrt{l'(l'+1)l(l+1)}\right. \\
&\qquad\left.+\frac{1+(-)^{L+l+l'}}{2}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1\end{pmatrix}\frac{(3l'-\eta'+1)(3\eta-l+1)}{2}\right] \\
&=(-)^{m'+1}\left[\frac{(2L+1)(2l'+1)(2l+1)}{4\pi}\right]^{\frac{1}{2}}\begin{pmatrix} l' & L & l \\ -m' & M & m\end{pmatrix}[l(l+1)l'(l'+1)]^{\frac{1}{2}}\frac{1+(-)^{L+l+l'}}{2}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1\end{pmatrix}
\end{aligned}
$$

where

$$\begin{aligned}
\int d\hat{\boldsymbol{r}}\boldsymbol{Y}^*_{l'\eta'm'}Y_{LM}\boldsymbol{Y}_{l\eta m} &= \frac{(-)^{m'+1}}{2}\left[\frac{2L+1}{4\pi}\right]^{\frac{1}{2}}\begin{pmatrix} l' & L & l \\ -m' & M & m \end{pmatrix} \\
&\times\Bigg[\begin{pmatrix} L & l & l' \\ 0 & 0 & 0 \end{pmatrix}(-)^{\frac{1}{2}(\eta'-l'+\eta-l)}\sqrt{(\eta'+l'+1)(\eta+l+1)} \\
&\quad +\frac{1+(-)^{L+l+l'}}{2}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}\sqrt{(3l'-\eta'+1)(3l-\eta+1)}\Bigg]
\end{aligned}$$

and

$(3l-\eta+1)(\eta+l+1) = 4l(l+1) \qquad \text{because}\eta = l\pm 1$

Therefore

$$\begin{aligned}
\langle l'm'|\overleftarrow{\nabla}\cdot Y_{LM}\overrightarrow{\nabla}|lm\rangle &= \langle l'm'|\left(\hat{\boldsymbol{r}}\frac{\overleftarrow{\partial}}{\partial r}-\frac{i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}}{r}\right)\cdot Y_{LM}\left(\hat{\boldsymbol{r}}\frac{\overrightarrow{\partial}}{\partial r}-\frac{i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}}{r}\right)|lm\rangle \\
&= \langle l'm'|Y_{LM}|lm\rangle\frac{\overleftarrow{\partial}}{\partial r}\frac{\overrightarrow{\partial}}{\partial r}+\langle l'm'|i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot Y_{LM}i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}|lm\rangle\frac{1}{r^2}
\end{aligned}$$

E.5.1 Reduced matrix element of $\langle l'm'|i\hat{\boldsymbol{r}}\times\boldsymbol{L}\cdot Y_{LM}i\hat{\boldsymbol{r}}\times\boldsymbol{L}|lm\rangle$

$$\begin{aligned}
&\langle l'm'|i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot Y_{LM}i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}|lm\rangle \\
&= (-)^{m'+1}\left[\frac{(2L+1)(2l'+1)(2l+1)}{4\pi}\right]^{\frac{1}{2}}\begin{pmatrix} l' & L & l \\ -m' & M & m \end{pmatrix}[l(l+1)l'(l'+1)]^{\frac{1}{2}}\frac{1+(-)^{L+l+l'}}{2}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}
\end{aligned}$$

From the Wigner-Eckart's theorem, one can get

$$\begin{aligned}
&\langle l'||i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot Y_L i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}||l\rangle \\
&= (-)^{l'+1}\left[\frac{(2L+1)(2l'+1)(2l+1)}{4\pi}\right]^{\frac{1}{2}}[l(l+1)l'(l'+1)]^{\frac{1}{2}}\frac{1+(-)^{L+l+l'}}{2}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}
\end{aligned}$$

L-J coupling

Using an useful formula for l-j coupling,

$$\langle l'j'||T_L||lj\rangle = (-)^{j+l'+L+1/2}(2j'+1)^{\frac{1}{2}}(2j+1)^{\frac{1}{2}}\begin{Bmatrix} j' & l' & 1/2 \\ l & j & L \end{Bmatrix}$$

then one can obtain

$$\begin{aligned}
&\langle l'j'||i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot Y_L i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}||lj\rangle \\
&= (-)^{j+L-1/2}\left[\frac{(2L+1)(2l'+1)(2j'+1)(2l+1)(2j+1)}{4\pi}\right]^{\frac{1}{2}}[l(l+1)l'(l'+1)]^{\frac{1}{2}}\frac{1+(-)^{L+l+l'}}{2} \\
&\qquad\times\begin{Bmatrix} j' & l' & 1/2 \\ l & j & L \end{Bmatrix}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1 \end{pmatrix}
\end{aligned}$$

$$
\begin{aligned}
\langle l'j'||i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot Y_L i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}||lj\rangle &= (-)^{j'+L+1/2}\frac{1}{2}\left[\frac{l(l+1)l'(l'+1)}{4\pi}\right]^{\frac{1}{2}}\frac{1+(-)^{L+l+l'}}{2} \\
&\times\Bigg[\sqrt{(4l'-2j'+1)(4l-2j+1)}\langle j',-1/2:j,1/2|L0\rangle \\
&\quad +(-)^{l+j+l'+j'}\sqrt{(6j'-4l'+1)(6j-4l+1)}\langle j',-3/2:j,3/2|L0\rangle\Bigg]
\end{aligned}
$$

where

$$
\begin{aligned}
&\left\{\begin{matrix} j' & l' & 1/2 \\ l & j & L\end{matrix}\right\}\begin{pmatrix} L & l & l' \\ 0 & 1 & -1\end{pmatrix} \\
&= (-)^{j+j'}\Bigg[\begin{pmatrix} L & j' & j \\ 0 & -\frac{1}{2} & \frac{1}{2}\end{pmatrix}\begin{pmatrix} l & j & \frac{1}{2} \\ 1 & -\frac{1}{2} & -\frac{1}{2}\end{pmatrix}\begin{pmatrix} l' & j' & \frac{1}{2} \\ 1 & -\frac{1}{2} & -\frac{1}{2}\end{pmatrix} \\
&\qquad -\begin{pmatrix} L & j' & j \\ 0 & -\frac{3}{2} & \frac{3}{2}\end{pmatrix}\begin{pmatrix} l & j & \frac{1}{2} \\ 1 & -\frac{3}{2} & \frac{1}{2}\end{pmatrix}\begin{pmatrix} l' & j' & \frac{1}{2} \\ 1 & -\frac{3}{2} & \frac{1}{2}\end{pmatrix}\Bigg] \\
&= -\frac{1}{2}\Bigg[\sqrt{\frac{(4l'-2j'+1)(4l-2j+1)}{(2j'+1)(2l'+1)(2j+1)(2l+1)}}\begin{pmatrix} j' & j & L \\ -\frac{1}{2} & \frac{1}{2} & 0\end{pmatrix} \\
&\qquad +(-)^{l+j+l'+j'}\sqrt{\frac{(6j'-4l'+1)(6j-4l+1)}{(2j'+1)(2l'+1)(2j+1)(2l+1)}}\begin{pmatrix} j' & j & L \\ -\frac{3}{2} & \frac{3}{2} & 0\end{pmatrix}\Bigg] \\
&= -\frac{(-)^{j'-j}}{2}\Bigg[\sqrt{\frac{(4l'-2j'+1)(4l-2j+1)}{(2j'+1)(2l'+1)(2j+1)(2l+1)(2L+1)}}\langle j',-1/2:j,1/2|L0\rangle \\
&\qquad +(-)^{l+j+l'+j'}\sqrt{\frac{(6j'-4l'+1)(6j-4l+1)}{(2j'+1)(2l'+1)(2j+1)(2l+1)(2L+1)}}\langle j',-3/2:j,3/2|L0\rangle\Bigg]
\end{aligned}
$$

E.6 Summary

$$\begin{aligned}\langle l'm'|Y_{LM}|lm\rangle &= (-)^{l'-m'}\begin{pmatrix} l' & L & l \\ -m' & M & m \end{pmatrix}\left[(-)^{l'}\sqrt{\frac{(2l'+1)(2L+1)(2l+1)}{4\pi}}\begin{pmatrix} l' & L & l \\ 0 & 0 & 0 \end{pmatrix}\right] \\ &= (-)^{l'-m'}\begin{pmatrix} l' & L & l \\ -m' & M & m \end{pmatrix}\langle l'||Y_L||l\rangle\end{aligned}$$

$$\langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot\hat{\boldsymbol{r}}|lm\rangle = \left[\left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\delta_{\lambda=L-1} - \left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\delta_{\lambda=L+1}\right]\langle l'm'|Y_{LM}|lm\rangle$$

$$\langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}|lm\rangle$$

$$= \frac{1+(-1)^{L+l+l'}}{2}\left[\left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\delta_{\lambda=L-1} + \left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\delta_{\lambda=L+1}\right]\frac{\sqrt{l(l+1)}\begin{pmatrix} l' & l & L \\ 0 & 1 & -1 \end{pmatrix}}{\begin{pmatrix} l' & L & l \\ 0 & 0 & 0 \end{pmatrix}}\langle l'm'|Y_{LM}|lm\rangle$$

$$\langle l'm'|i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot\boldsymbol{Y}_{L\lambda M}|lm\rangle$$

$$= -\left[(L+1)\left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\delta_{\lambda=L-1} + L\left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\delta_{\lambda=L+1}\right]\langle l'm'|Y_{LM}|lm\rangle - \langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\boldsymbol{L}|lm\rangle$$

Therefore

$$\langle l'm'|\overleftarrow{\nabla}\cdot\boldsymbol{Y}_{L\lambda M} + \boldsymbol{Y}_{L\lambda M}\cdot\overrightarrow{\nabla}|lm\rangle$$

$$= \langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot\hat{\boldsymbol{r}}|lm\rangle\left[\frac{\overleftarrow{\partial}}{\partial r} + \frac{\overrightarrow{\partial}}{\partial r}\right] + \left[\langle l'm'|i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot\boldsymbol{Y}_{L\lambda M}|lm\rangle + \langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}|lm\rangle\right]\frac{1}{r}$$

$$= \begin{cases} (\lambda=L-1): & \left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\langle l'm'|Y_{LM}|lm\rangle\left[\frac{\overleftarrow{\partial}}{\partial r} + \frac{\overrightarrow{\partial}}{\partial r}\right] - (L+1)\left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\langle l'm'|Y_{LM}|lm\rangle\frac{1}{r} \\ (\lambda=L+1): & -\left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\langle l'm'|Y_{LM}|lm\rangle\left[\frac{\overleftarrow{\partial}}{\partial r} + \frac{\overrightarrow{\partial}}{\partial r}\right] - L\left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\langle l'm'|Y_{LM}|lm\rangle\frac{1}{r} \end{cases}$$

$$\langle l'm'|\overleftarrow{\nabla}\cdot\boldsymbol{Y}_{L\lambda M} - \boldsymbol{Y}_{L\lambda M}\cdot\overrightarrow{\nabla}|lm\rangle$$

$$= \langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot\hat{\boldsymbol{r}}|lm\rangle\left[\frac{\overleftarrow{\partial}}{\partial r} - \frac{\overrightarrow{\partial}}{\partial r}\right] + \left[\langle l'm'|i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot\boldsymbol{Y}_{L\lambda M}|lm\rangle - \langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}|lm\rangle\right]\frac{1}{r}$$

$$= \begin{cases} (\lambda=L-1): & \left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\langle l'm'|Y_{LM}|lm\rangle\left[\frac{\overleftarrow{\partial}}{\partial r} - \frac{\overrightarrow{\partial}}{\partial r}\right] \\ & -\left[(L+1)\left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\langle l'm'|Y_{LM}|lm\rangle + 2\langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\boldsymbol{L}|lm\rangle|_{\lambda=L-1}\right]\frac{1}{r} \\ (\lambda=L+1): & -\left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\langle l'm'|Y_{LM}|lm\rangle\left[\frac{\overleftarrow{\partial}}{\partial r} - \frac{\overrightarrow{\partial}}{\partial r}\right] \\ & -\left[L\left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\langle l'm'|Y_{LM}|lm\rangle + 2\langle l'm'|\boldsymbol{Y}_{L\lambda M}\cdot i\hat{\boldsymbol{r}}\times\boldsymbol{L}|lm\rangle|_{\lambda=L+1}\right]\frac{1}{r} \end{cases}$$

If one uses an useful formula,

$$\langle l'j'||T_L||lj\rangle = (-)^{j+l'+L+1/2}(2j'+1)^{1/2}(2j+1)^{1/2}\left\{\begin{array}{ccc} j' & l' & \frac{1}{2} \\ l & j & L \end{array}\right\}\langle l'||T_L||l\rangle$$

and also uses the Wigner-Eckart's formula, then one can get

$$\begin{aligned}
&\langle l'j'||\overleftarrow{\nabla}\cdot\boldsymbol{Y}_{L\lambda}+\boldsymbol{Y}_{L\lambda}\cdot\overrightarrow{\nabla}||lj\rangle \\
&=\langle l'j'||\boldsymbol{Y}_{L\lambda}\cdot\hat{\boldsymbol{r}}||lj\rangle\left[\frac{\overleftarrow{\partial}}{\partial r}+\frac{\overrightarrow{\partial}}{\partial r}\right]+\left[\langle l'j'||i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot\boldsymbol{Y}_{L\lambda}||lj\rangle+\langle l'j'||\boldsymbol{Y}_{L\lambda}\cdot i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}||lj\rangle\right]\frac{1}{r} \\
&=\begin{cases}
(\lambda=L-1): & \left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\langle l'j'||Y_L||lj\rangle\left[\frac{\overleftarrow{\partial}}{\partial r}+\frac{\overrightarrow{\partial}}{\partial r}\right]-(L+1)\left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\langle l'j'||Y_L||lj\rangle\frac{1}{r} \\
(\lambda=L+1): & -\left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\langle l'j'||Y_L||lj\rangle\left[\frac{\overleftarrow{\partial}}{\partial r}+\frac{\overrightarrow{\partial}}{\partial r}\right]-L\left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\langle l'j'||Y_L||lj\rangle\frac{1}{r}
\end{cases}
\end{aligned}$$

$$\begin{aligned}
&\langle l'j'||\overleftarrow{\nabla}\cdot\boldsymbol{Y}_{L\lambda}-\boldsymbol{Y}_{L\lambda}\cdot\overrightarrow{\nabla}||lj\rangle \\
&=\langle l'j'||\boldsymbol{Y}_{L\lambda}\cdot\hat{\boldsymbol{r}}||lj\rangle\left[\frac{\overleftarrow{\partial}}{\partial r}-\frac{\overrightarrow{\partial}}{\partial r}\right]+\left[\langle l'j'||i\hat{\boldsymbol{r}}\times\overleftarrow{\boldsymbol{L}}\cdot\boldsymbol{Y}_{L\lambda}||lj\rangle-\langle l'j'||\boldsymbol{Y}_{L\lambda}\cdot i\hat{\boldsymbol{r}}\times\overrightarrow{\boldsymbol{L}}||lj\rangle\right]\frac{1}{r} \\
&=\begin{cases}
(\lambda=L-1): & \left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\langle l'j'||Y_L||lj\rangle\left[\frac{\overleftarrow{\partial}}{\partial r}-\frac{\overrightarrow{\partial}}{\partial r}\right] \\
& -\left[(L+1)\left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\langle l'j'||Y_L||lj\rangle+2\langle l'j'||\boldsymbol{Y}_{L\lambda}\cdot i\hat{\boldsymbol{r}}\times\boldsymbol{L}||lj\rangle|_{\lambda=L-1}\right]\frac{1}{r} \\
(\lambda=L+1): & -\left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\langle l'j'||Y_L||lj\rangle\left[\frac{\overleftarrow{\partial}}{\partial r}-\frac{\overrightarrow{\partial}}{\partial r}\right] \\
& -\left[L\left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\langle l'j'||Y_L||lj\rangle+2\langle l'j'||\boldsymbol{Y}_{L\lambda}\cdot i\hat{\boldsymbol{r}}\times\boldsymbol{L}||lj\rangle|_{\lambda=L+1}\right]\frac{1}{r}
\end{cases}
\end{aligned}$$

where

$$\langle l'j'||Y_L||lj\rangle = (-)^{j'+L-1/2}\left(\frac{1+(-)^{L+l+l'}}{2}\right)\sqrt{\frac{(2j'+1)(2j+1)}{4\pi}}\langle j1/2:j'-1/2|L0\rangle$$

$$\begin{aligned}
&\langle l'j'||\boldsymbol{Y}_{L\lambda}\cdot i\hat{\boldsymbol{r}}\times\boldsymbol{L}||lj\rangle \\
&=(-)^{j+L+1/2}\frac{1+(-1)^{L+l+l'}}{2}\sqrt{\frac{l(l+1)}{2(2j+1)}}\sqrt{\frac{(2j'+1)(2j+1)}{4\pi}}\left[\left(\frac{L+1}{2L+1}\right)^{\frac{1}{2}}\delta_{\lambda=L-1}+\left(\frac{L}{2L+1}\right)^{\frac{1}{2}}\delta_{\lambda=L+1}\right] \\
&\times\left\{(-)^{l+l'+1}\sqrt{2l-j+1/2}\langle j1/2:j'1/2|L1\rangle+(-)^{j+j'+1}\sqrt{3j-2l+1/2}\langle j3/2:j'-1/2|L1\rangle\right\}
\end{aligned}$$

Appendix F

Feynman diagram and Feynman rule

F.1 Feynman rule in the Relativistic formalism

The feynman rule is defined so as to express S-matrix graphically. S-matrix is given by

$$S_{fi} = \langle f| \sum_{n=0}^{\infty} S^{(n)} |i\rangle \qquad S^{(n)} \text{ : n-th order S-matrix in perturbation theory.}$$

$$S^{(n)} = \frac{(-)^n}{n!} \mathrm{T} \left[\int d^4x_1 \cdots \int d^4x_n \{\mathcal{H}_I(x_1) \cdots \mathcal{H}_I(x_n)\} \right]$$

where $\mathcal{H}_I (= \mathcal{L}_I)$ is interaction Hamiltonian.(equal to the interaction Lagrangian.) S-matrix is the value which is related to the differential cross section(Exercise (I)). Interaction Hamiltonian depends on the kinds of field, for example, the interaction Hamiltonian of electro-magnetic field is given by

$$\mathcal{H}_I(x) = ieN \left[\bar{\psi}(x) \gamma^\mu \psi(x) A_\mu(x) \right]$$

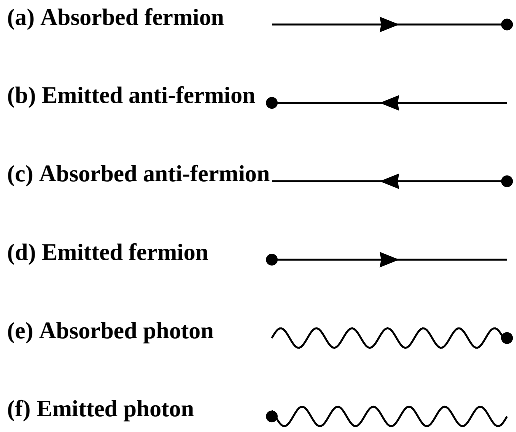
where ψ is the Dirac spinor field operator and A_μ is the vector field operator of the electro-magnetic field. Both ψ and A_μ can be expressed by a creation and an anihilation operators of fermion(anti-fermion) and photon respectively.

$$\psi(x) = \sum_s \int d^4p \left[c_s(p) u_s(p) e^{-ipx} + d_s^\dagger(p) v_s(p) e^{+ipx} \right] = \psi^+(x) + \psi^-(x)$$

$$\bar{\psi}(x) = \sum_s \int d^4p \left[c_s^\dagger(p) \bar{u}_s(p) e^{+ipx} + d_s(p) \bar{v}_s(p) e^{-ipx} \right] = \bar{\psi}^-(x) + \bar{\psi}^+(x)$$

$$A_\mu(x) = \sum_r \int d^4k \left[\epsilon_\mu^r a_r(k) e^{-ikx} + \epsilon_\mu^r a_r^\dagger(k) e^{+ikx} \right] = A_\mu^+(x) + A_\mu^-(x)$$

(a)ψ^+ means "absorbed fermion", (b)ψ^- means "emitted anti-fermion", (c)$\bar{\psi}^+$ means "absorbed anti-fermion", (d)ψ^- means "emitted fermion", (e)A_μ^+ means "abosorbed photon", and (f)A_μ^- means "emitted photon" respectively.



The most basic feynman rules can be defined here. (a)-(f) correspond to each diagrams as seen in the right figures respectively. One should pay attention to the direction of arrow in figures means the momentum direction. Notice that the definition of the arrow direction in the feynman diagram may be different for each any textbooks.
For example, the 1-st order S-matrix includes

$$S^{(1)} \ni ie \int d^4xN \left[\bar{\psi}^+\gamma^\mu\psi^+A_\mu^-\right].$$

This term corresponds to the diagram of Figure.F.1.

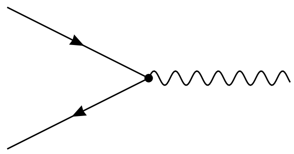


Figure F.1:

Exercise(II)

Draw the diagram corresponds to

$$ie \int d^4xN \left[\bar{\psi}^+\gamma^\mu\psi^-A_\mu^+\right].$$

F.1.1 Propagator and Feynman rule

Propagators mean the exchanging vertual particles, and are equivalent to the "potential" or "interaction". For example, "vertual photon" is equal to the "electro-magnetic intearction", "pion" is equal to the "one-pion exchange potential" which is related to the nuclear force. "Yukawa force" is related to the "scalar

Propagators **propagate** properties of particles, quantum number, momentum, mass, and so on, between channels.

Typycal propagators can be given by

$$\text{(a)}\quad iS_F(x-x') = \langle 0|T\left[\psi(x)\psi^\dagger(x')\right]|0\rangle = \frac{i}{(2\pi)^4}\int d^4p\frac{\gamma^\mu p_\mu + m}{p^2-m^2+i\epsilon}e^{-ip(x-x')} \qquad \text{Fermion}$$

$$\text{(b)}\quad i\Delta_F(x-x') = \langle 0|T\left[\phi(x)\phi^\dagger(x')\right]|0\rangle = \frac{i}{(2\pi)^4}\int d^4k\frac{1}{k^2-m^2+i\epsilon}e^{-ik(x-x')} \qquad \text{Scalar Boson}$$

$$\text{(c)}\quad iD_{F0}^{\mu\nu}(x-x') = \langle 0|T\left[A^\mu(x)A^\nu(x')\right]|0\rangle = \frac{i}{(2\pi)^4}\int d^4k\frac{-g^{\mu\nu}}{k^2-m^2+i\epsilon}e^{-ik(x-x')} \quad \text{Massless Vector Boson}$$

$$\text{(d)}\quad iD_{FM}^{\mu\nu}(x-x') = \langle 0|T\left[A^\mu(x)A^\nu(x')\right]|0\rangle = \frac{i}{(2\pi)^4}\int d^4k\frac{-g^{\mu\nu}+\frac{k^\mu k^\nu}{m^2}}{k^2-m^2+i\epsilon}e^{-ik(x-x')} \qquad \text{Vector Boson}$$

Fermion propagator satisfies Dirac-type equation, and also Boson propagator satisfies Klein-Gordon-type equation. Sometimes this is the definition of the propagator. In the non-relativistic formalism, propagator is called "Green's function" . "Green's function" satisfies Schrodinger-like equation. This is the definition of the Green's function.

F.1.2 Application of the Feynman rules to the 2nd order S-matrix

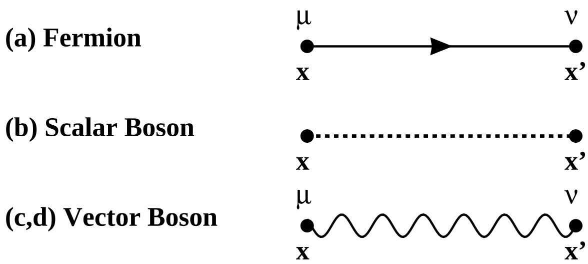
In order to apply the Feynman rules to the 2nd order S-matrix, one should study **Wick's theorem**. Wick's theorem is well known thorem and often used not only in the relativistic formalism but also in the non-relativistic 2nd quantized field theory. But because wick's theorem is rather comlicated, and its proof is defficult, so I only introduce this theorem.

Exercise(III)

Make sure that each paorgators satisfy each equations.

Feynman rules for each propagators

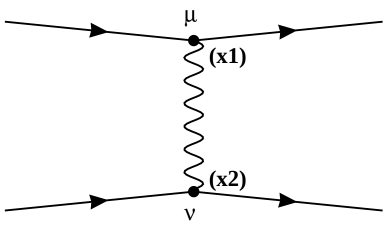
Here the Feynman rules for each propagators (a)-(d) can be defined as right figures.



By using Wick's theorem,

$$S^{(2)} \ni -\frac{e^2}{2}\int\int d^4x_1 d^4x_2 N\left[\left(\bar{\psi}^-\gamma^\mu\psi^+\right)_{x_1}\left(\bar{\psi}^-\gamma^\nu\psi^+\right)_{x_2}\right] iD_{F,\mu\nu}(x_1-x_2)$$

is included. This term corresponds to a diagram of right figure.



Exercise(IV)

Study Wick's theorem by using some textbooks of the quantum field theory.

Exercise(V)

By using Wick's theorem, derive all Feynman diagrams in the 2nd order S-matrix.

F.1.3 Propagator and Potential

As the previous subsection, the propagator is related to the potential in the static limit. In the static limit, the (scalar boson) propagator in the momentum space is given by

$$\frac{1}{\boldsymbol{k}^2+m^2}$$

The Fourier transformation of this propagator yields Yukawa potential.

$$\int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{kr}} \frac{1}{\boldsymbol{k}^2+m^2} = \frac{1}{4\pi}\frac{e^{-mr}}{r}$$