One-body operator in second quantization

One-body operators depend upon one radial coordinate $\mathbf{r}$ only. In second quantization a one-body operator $\hat{M}$ can be written as,

$$\hat{M} = \sum_{pq} \langle p|\hat{M}|q\rangle c_p^\dagger c_q$$

where p and q run over all single-particle states (particle- as well as hole-states).

To proof that this is correct we will evaluate the matrix element of $\hat{M}$ between two single-particle states, i. e. (A+1)-states of the form $|i\rangle = c_i^\dagger|0\rangle$ for which $n_i = 0$. The final result of this calculation sould be that we get the matrix element itself again.

We then evaluate

$$
\begin{aligned}
\langle i|\hat{M}|j\rangle =& \langle 0|c_i\hat{M}c_j^\dagger|0\rangle = \sum_{pq}\langle p|\hat{M}|q\rangle\langle 0|c_ic_p^\dagger c_qc_j^\dagger|0\rangle \\
=& \sum_{pq}\langle p|\hat{M}|q\rangle\langle 0|\overbrace{c_ic_p^\dagger}\overbrace{c_qc_j^\dagger} + \overbrace{c_ic_j^\dagger}\overbrace{c_p^\dagger c_q}|0\rangle \\
=& \sum_{pq}\langle p|\hat{M}|q\rangle\Big[(1-n_i)\delta_{ip}(1-n_j)\delta_{qj} + (1-n_i)\delta_{ij}n_p\delta_{pq}\Big] \\
=& (1-n_i)(1-n_j)\langle i|\hat{M}|j\rangle + (1-n_i)\delta_{ij}\sum_p n_p\langle p|\hat{M}|p\rangle
\end{aligned}
\tag{1}
$$

and we see that with $n_i = n_j = 0$ we get the matrix element we needed, i. e. $\langle i|\hat{M}|j\rangle$, but that there is also another contribution which appears only when $i = j$. This corresponds to the sum of the mean values of $\hat{M}$ over all hole states. It is the interaction of the particles in the A-nucleon core among themselves, leaving the particle in the (A+1)-nucleus untouched. This term is called "core polarization".

To avoid polarization effects one defines

$$\hat{M} = \sum_{pq} \langle p|\hat{M}|q\rangle : c_p^\dagger c_q :$$

that is, one assumes that $\hat{M}$ itself includes polarization. One sees that this avoids the core polarization term, since one cannot contract the indeces p and q (i. e. the term δ_{pq} in Eq. (1)).

Two-body operator

To avoid effects related to the interaction of the particles in the core, as it was the core polarization effect in the one-particle case above, one defines the two-body operator in second quantization in normal form, i. e. as,

$$\hat{M} = \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{M} | \gamma\delta \rangle : c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma : \tag{2}$$

and evaluate the matrix element of this operator between antisymmetrized two-particle states, i. e. states in the (A+2)-nucleus. Our aim is to show that this procedure will indeed provide the antisymmetrized matrix element. In this context

The antisymmetrized two-particle states are,

$$|ij\rangle_a = c_i^\dagger c_j^\dagger |0\rangle \Longrightarrow {}_a\langle ij| = \langle 0|(c_i^\dagger c_j^\dagger)^\dagger = \langle 0|c_j c_i \tag{7.41}$$

and the matrix element is,

$${}_a\langle ij|\hat{M}|kl\rangle_a = \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta|\hat{M}|\gamma\delta\rangle \langle 0|c_j c_i : c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma : c_k^\dagger c_l^\dagger |0\rangle \tag{7.42}$$

Since the mean value of operators in normal form vanishes, the terms that survive contain only contractions. They are,

$$c_j c_i : c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma : c_k^\dagger c_l^\dagger = \left[\overbrace{c_i c_\alpha^\dagger}\,\overbrace{c_j c_\beta^\dagger} - \overbrace{c_i c_\beta^\dagger}\,\overbrace{c_j c_\alpha^\dagger}\right]\left[\overbrace{c_\gamma c_k^\dagger}\,\overbrace{c_\delta c_l^\dagger} - \overbrace{c_\gamma c_l^\dagger}\,\overbrace{c_\delta c_k^\dagger}\right] \tag{7.43}$$

which give,

$$\begin{aligned}
{}_a\langle ij|\hat{M}|kl\rangle_a =& \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta|\hat{M}|\gamma\delta\rangle \Big[(1-n_i)\delta_{i\alpha}(1-n_j)\delta_{j\beta} - (1-n_i)\delta_{i\beta}(1-n_j)\delta_{j\alpha}\Big] \\
&\times \Big[(1-n_k)\delta_{k\gamma}(1-n_l)\delta_{l\delta} - (1-n_k)\delta_{k\delta}(1-n_l)\delta_{l\gamma}\Big] \\
=&(1-n_i)(1-n_j)(1-n_k)(1-n_l)\Big[\langle ij|\hat{M}|kl\rangle_a - \langle ji|\hat{M}|kl\rangle_a\Big] \\
&-(1-n_i)(1-n_j)(1-n_k)(1-n_l)\Big[\langle ij|\hat{M}|lk\rangle_a - \langle ji|\hat{M}|lk\rangle_a\Big]
\end{aligned} \tag{7.44}$$

The matrix element antisymmetrized to the right only becomes,

$$\langle ji|\hat{M}|kl\rangle_a = \langle ji|\hat{M}\left[|kl\rangle - |lk\rangle\right] = \langle ij|\hat{M}\left[|lk\rangle - |kl\rangle\right] = -\langle ij|\hat{M}|kl\rangle_a$$

and Eq. (3) becomes,

$${}_a\langle ij|\hat{M}|kl\rangle_a = (1-n_i)(1-n_j)(1-n_k)(1-n_l)\,{}_a\langle ij|\hat{M}|kl\rangle_a$$

The Hamiltonian becomes,

$$H = \sum_{\alpha\beta}\langle\alpha|T|\beta\rangle c_\alpha^\dagger c_\beta + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\gamma\delta\rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma.$$

II

Random Phase approximation and Tamm-Dancoff approximation

May 6, 2013

One-body operators depend upon one radial coordinate $\mathbf{r}$ only. In second quantization a one-body operator $\hat{M}$ can be written as,

$$\hat{M} = \sum_{pq} \langle p|\hat{M}|q\rangle c_p^\dagger c_q = \sum_{pq} \langle p|\hat{M}|q\rangle [: c_p^\dagger c_q : + \overbrace{c_p^\dagger c_q}]$$

$$\begin{aligned}
\langle i|\hat{M}|j\rangle =& \langle 0|c_i \hat{M} c_j^\dagger|0\rangle = \sum_{pq} \langle p|\hat{M}|q\rangle \langle 0|c_i c_p^\dagger c_q c_j^\dagger|0\rangle \\
=& \sum_{pq} \langle p|\hat{M}|q\rangle \langle 0| \overbrace{c_i c_p^\dagger} \overbrace{c_q c_j^\dagger} + \overbrace{c_i c_j^\dagger} \overbrace{c_p^\dagger c_q} |0\rangle \\
=& \sum_{pq} \langle p|\hat{M}|q\rangle \left[(1-n_i)\delta_{ip}(1-n_j)\delta_{qj} + (1-n_i)\delta_{ij} n_p \delta_{pq}\right] \\
=& (1-n_i)(1-n_j)\langle i|\hat{M}|j\rangle + (1-n_i)\delta_{ij} \sum_p n_p \langle p|\hat{M}|p\rangle
\end{aligned}$$

Two-body operator

$$\hat{M} = \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta|\hat{M}|\gamma\delta\rangle : c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma :$$

We found that to avoid core excitations the one-body operator should be defined in terms of normal products. That is to use $: c^\dagger_\alpha c_\beta :$ instead of $c^\dagger_\alpha c_\beta$. It was due to this that we wrote the two-body operator in normal form also. But in doing so we bypassed what maybe an important physics. And indeed there is an important

$$H = \sum_{\alpha\beta} \langle \alpha | T | \beta \rangle c^\dagger_\alpha c_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma .$$

Converting to normal form one gets,

$$H = \sum_{\alpha\beta} \langle \alpha | T | \beta \rangle (: c^\dagger_\alpha c_\beta : + \overbrace{c^\dagger_\alpha c_\beta}) + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle [: c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma :$$
$$+ : c^\dagger_\alpha c_\gamma : \overbrace{c^\dagger_\beta c_\delta} - : c^\dagger_\alpha c_\delta : \overbrace{c^\dagger_\beta c_\gamma} - : c^\dagger_\beta c_\gamma : \overbrace{c^\dagger_\alpha c_\delta} + : c^\dagger_\beta c_\delta : \overbrace{c^\dagger_\alpha c_\gamma}$$
$$+ \overbrace{c^\dagger_\alpha c_\gamma}\, \overbrace{c^\dagger_\beta c_\delta} - \overbrace{c^\dagger_\alpha c_\delta}\, \overbrace{c^\dagger_\beta c_\gamma}]$$

Hartree-Fock potential

After some algebra to be performed,

$$H = E_0 + H_{HF} + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\gamma\delta\rangle : c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma :$$

where

$$E_0 = \sum_\alpha n_\alpha \langle\alpha|T|\alpha\rangle + \frac{1}{2}\sum_{\alpha\beta}\langle\alpha\beta|V|\alpha\beta\rangle_a \tag{9}$$

This is the kinetic energy of particles in the occupied states plus the interaction between particles placed in any pair of levels of the representation. It is the energy carried by the core, as can also be seen by noticing that $E_0 = \langle 0|H|0\rangle$.

The one-body Hamiltonian is

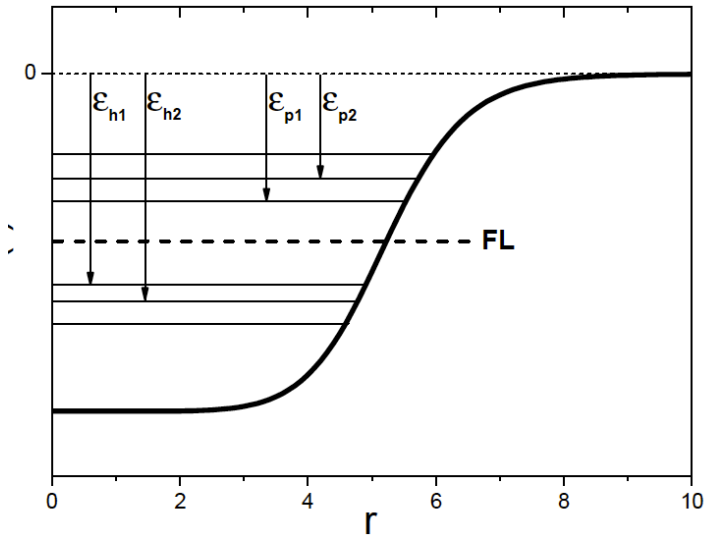
$$H_{HF} = \sum_{\alpha\beta}\left(\langle\alpha|T|\beta\rangle + \sum_\gamma n_\gamma \langle\alpha\gamma|V|\beta\gamma\rangle_a\right) : c_\alpha^\dagger c_\beta :$$

In this Hamiltonian the levels α and β include all states of the representation. These are the levels that we will occupied by particles which eventually will be added to the

The one-body Hamiltonian is

$$H_{HF} = \sum_{\alpha\beta} \left(\langle \alpha | T | \beta \rangle + \sum_{\gamma} n_\gamma \langle \alpha\gamma | V | \beta\gamma \rangle_a \right) : c_\alpha^\dagger c_\beta :$$

In this Hamiltonian the levels α and β include all states of the representation. These are the levels that we will occupied by particles which eventually will be added to the core. One thus sees that H_{HF} contains the core excitations through the interaction of particles in all occupied states (called $|\gamma\rangle$ in H_{HF}) with the rest of the particles (including those in the core). The Hamiltonian H_{HF}, which is called the Hartree-Fock Hamiltonian, thus corresponds to the core excitation which in the one-body case were assumed to be contained in the renormalized operators.



The diagonalization of H_{HF} provides the Hartree-Fock representation. This is not a very easy task because it is not a linear problem. To see this we write H_{HF} in Dirac notation, i.e.

$$H_{HF} = \sum_{\alpha\beta} |\alpha\rangle \left(\langle\alpha|T|\beta\rangle + \sum_{\gamma} n_\gamma \langle\alpha\gamma|V|\beta\gamma\rangle_a \right) \langle\beta|$$

and the Hartree-Fock representation will be defined by the eigenvectors $\{|i\rangle\}$ given by,

$$H_{HF}|i\rangle = \varepsilon_i |i\rangle$$

To solve this eigenvalue problem we multiply by $\langle\alpha|$ from the left to get,

$$\sum_{\beta} \left(\langle\alpha|T|\beta\rangle + \sum_{\gamma} n_\gamma \langle\alpha\gamma|V|\beta\gamma\rangle_a \right) \langle\beta|i\rangle = \varepsilon_i \langle\alpha|i\rangle$$

and the eigenvectors are obtained by imposing the normalization condition,

$$|i\rangle = \sum_{\alpha} \langle\alpha|i\rangle |\alpha\rangle, \quad \langle i|i\rangle = 1$$

Within the representation $\{|i\rangle\}$ it should be

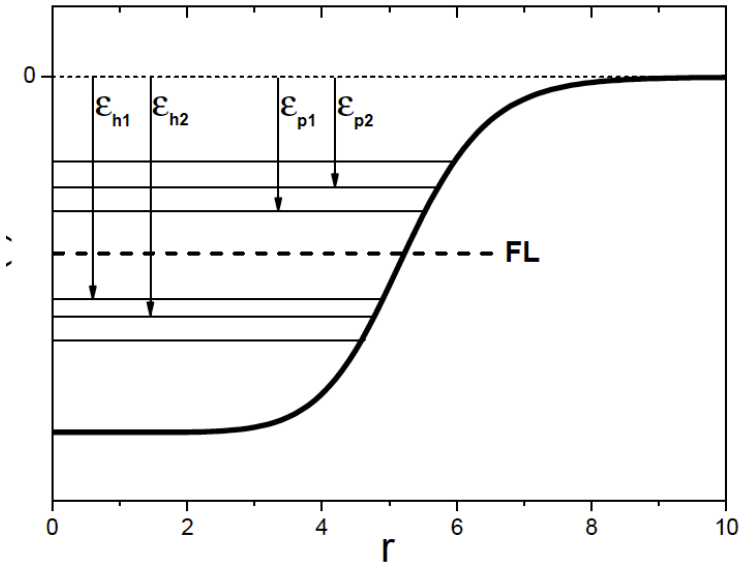
$$\langle j|H_{HF}|i\rangle = \varepsilon_i \delta_{ij}$$

Random Phase Approximation (RPA)

In this Section we will study the dynamics of the (A+2)- and (A-2)-nuclei, that is of two nucleons added or substracted from the core. For this we will write the Hamiltonian in the Hartre-Fock representation which we will label with greek as well as latin letters. It is,

$$H = \sum_{\alpha} \varepsilon_{\alpha} : c_{\alpha}^{\dagger} c_{\alpha} : + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle : c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma} : \qquad (7)$$

where ε_{α} is the Hartrre-Fock single-particle energy. The constant energy E_0, Eq. (6), is not included because all eigenvalues of the Hamiltonian (7) will be referred to the core and, therefore, E_0 plays no role.



To obtain the two-particle energies we evaluate the commutator,

$$\begin{aligned}\left[H, c_\alpha^\dagger c_\beta^\dagger\right] =& \sum_i \varepsilon_i \left[: c_i^\dagger c_i :, c_\alpha^\dagger c_\beta^\dagger\right] + \frac{1}{2}\sum_{ijkl}\langle ij|V|kl\rangle \left[: c_i^\dagger c_j^\dagger c_l c_k :, c_\alpha^\dagger c_\beta^\dagger\right] \\ =&(\varepsilon_\alpha + \varepsilon_\beta) c_\alpha^\dagger c_\beta^\dagger + (1 - n_\alpha - n_\beta)\sum_{i<j}\langle ij|V|\alpha\beta\rangle_a c_i^\dagger c_j^\dagger \\ &+ \sum_{i<j}\sum_l \langle ij|V|\beta l\rangle_a : c_i^\dagger c_j^\dagger c_\alpha^\dagger c_l : - \sum_{i<j}\sum_l \langle ij|V|\alpha l\rangle_a : c_i^\dagger c_j^\dagger c_\beta^\dagger c_l :\end{aligned} \tag{8}$$

One sees in this equation that the two-particle creation operators are mixed with three-particle one-hole excitations, that is with core excitation components. In the Random Phase Approximation (RPA) one neglects the core excitations, that is terms of the form $\langle n_2| : c_i^\dagger c_j^\dagger c_\alpha^\dagger c_l : |0\rangle$, because they are supposed to generate states which lie high in the spectrum, thus having little influence over the low-lying two-particle

RPA equation

one gets,

$$\langle n_2|\left[H, c_\alpha^\dagger c_\beta^\dagger\right]|0\rangle = (E_{n_2} - E_0)\langle n_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle$$
$$= (\varepsilon_\alpha + \varepsilon_\beta)\langle n_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle + (1 - n_\alpha - n_\beta)\sum_{i<j}\langle ij|V|\alpha\beta\rangle_a\langle n_2|c_i^\dagger c_j^\dagger|0\rangle$$

which is the RPA equation. The term $1 - n_\alpha - n_\beta$ in the RPA equations shows that one can place two particles above the Fermi level, in which case it is $1 - n_\alpha - n_\beta = 1$, or below it ($1 - n_\alpha - n_\beta$ = -1). These two forms of excitations are mixed to each other, given rise to the so-called RPA correlations. This also implies that within the RPA one evaluates simultaneously the (A+2)- and (A-2)-systems and, therefore, there is an influence of one system upon the other.

With $\omega_{n_2} = E_{n_2} - E_0$ the RPA equation can be written in matrix form as

$$\omega_{n_2} \begin{pmatrix} X_{n_2} \\ Y_{n_2} \end{pmatrix} = \begin{pmatrix} A & B \\ -C & -D \end{pmatrix} \begin{pmatrix} X_{n_2} \\ Y_{n_2} \end{pmatrix} \tag{10}$$

where $X_{n_2}(\alpha\beta) = \langle n_2 | c_\alpha^\dagger c_\beta^\dagger | 0 \rangle$ with α and β particle states and $Y_{n_2}(\alpha\beta) = \langle n_2 | c_\alpha^\dagger c_\beta^\dagger | 0 \rangle$ but with α and β hole states. In the same fashion the indices of A are all particle states and the indices of D are all hole states. Instead in the matrices B and C the indices are mixed. For instance $C(\alpha\beta\gamma\delta) = \langle \gamma\delta | V | \alpha\beta \rangle_a$, where α and β are hole states while γ and δ are particle states. Notice that the minus sign in front of the matrices C and D comes from the factor $1 - n_\alpha - n_\beta$ in Eq. (9). Due to this, the RPA matrix (10) is not Hermitian and, therefore, the energies ω_{n_2} can become complex quantities.

The two-particle state can be written as,

$$|n_2\rangle = \sum_{\alpha\leq\beta} X(\alpha\beta, n_2) c^\dagger_\alpha c^\dagger_\beta |0\rangle$$

and multiplying by $\langle m_2|$ one gets

$$\delta_{n_2 m_2} = \sum_{\alpha\leq\beta} X(\alpha\beta, n_2) \langle m_2| c^\dagger_\alpha c^\dagger_\beta |0\rangle$$

since the basis elements form and independent set one finds, comparing with Eq. (13),

$$X(\alpha\beta, n_2) = (1 - n_\alpha - n_\beta) \langle n_2| c^\dagger_\alpha c^\dagger_\beta |0\rangle^*$$

which is the RPA wave function amplitude.

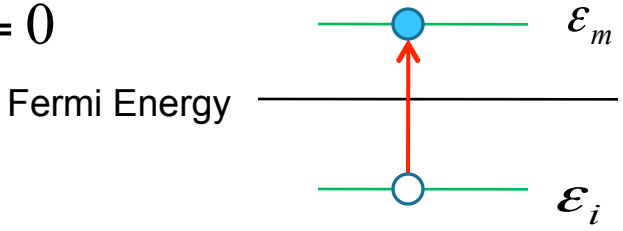
Closed shell: 1p-1h correlation

p-h phonon operator

$$Q^{+} = \sum_{m,i} X_{mi} a_m^{+} a_i - \sum_{m,i} Y_{mi} a_i^{+} a_m$$

$$\left[H, Q^{+}\right] = \hbar\omega Q^{+}$$

$$Q\left|RPA\right\rangle = 0$$



RPA equation

$$\begin{pmatrix} A & B \\ B^{*} & A^{*} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \hbar\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix}$$

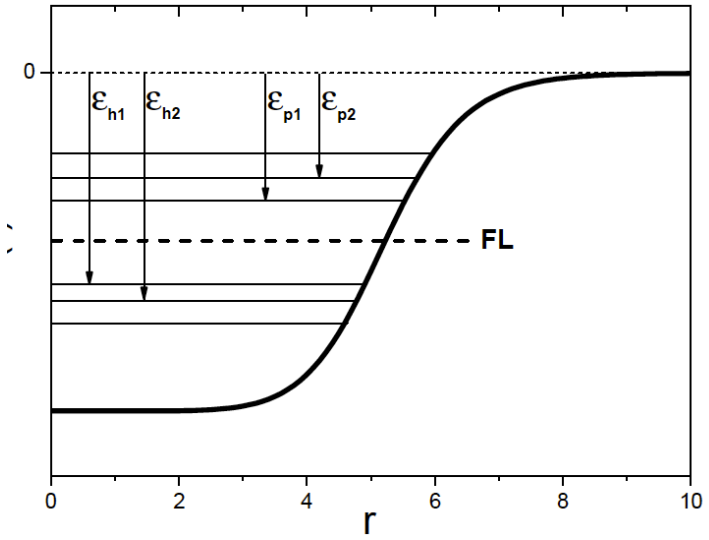
$$A_{mi\,nj} = (\varepsilon_m - \varepsilon_i)\delta_{mn}\delta_{ij} + \tilde{v}_{nijm}$$

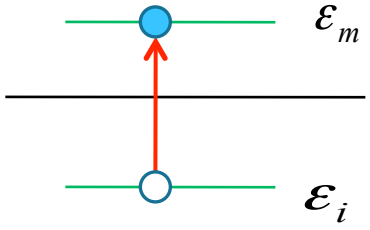
$$B_{mi\,nj} = \tilde{v}_{mnij}$$

Tamm-Damkoff Approximation (TDA)

The difference between TDA and RPA is that we use

- The simple particle-hole vacuum |HF> in TDA
- The correlated ground state in the RPA





Tamm-Damkoff Approximation (TDA)

We will concentrate in the shell model in this course, and here one has either two-particle or two-hole excitations, and the (A+2) and (A-2) systems are independent of each other. The shell model cases are actually particular cases of the RPA since one gets them by imposing the condition that only particles can occupied particle states and only holes can occupied hole states. This is called Tamm-Damkoff approximation (TDA).

This approximation implies that the matrices B and C vanish in Eq. (10). The particle- and hole-states decoupled and the RPA equation transforms in two TDA equations, one for particle states, i. e.

$$\omega_{n_2} X_{n_2} = A X_{n_2}$$

and the other one for hole states,

$$-\omega_{n_2} Y_{n_2} = D Y_{n_2}$$

Since the matrices A and D are Hermitians the energies are real, as they should be.

TDA equation

$$\begin{aligned}\langle n_2|\left[H, c_\alpha^\dagger c_\beta^\dagger\right]|0\rangle =&(E_{n_2}-E_0)\langle n_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle \\ =&(\varepsilon_\alpha+\varepsilon_\beta)\langle n_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle+\sum_{i<j}\langle ij|V|\alpha\beta\rangle_a\langle n_2|c_i^\dagger c_j^\dagger|0\rangle\end{aligned} \tag{14}$$

which is the TDA equation. It is also the shell model equation, which we will apply in the next Chapter.

For holes

$$\begin{aligned}\langle n_2|\left[H, c_\alpha c_\beta\right]|0\rangle =&(E_{n_2}-E_0)\langle n_2|c_\alpha c_\beta|0\rangle \\ =&-(\varepsilon_\alpha+\varepsilon_\beta)\langle n_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle+\sum_{i<j}\langle ij|V|\alpha\beta\rangle_a\langle n_2|c_i c_j|0\rangle\end{aligned}$$

The TDA wave function can be written in the two-particle basis $\{c_\alpha^\dagger c_\beta^\dagger|0\rangle\}$, where it should be $\alpha < \beta$ because the states $\alpha\beta$ and $\beta\alpha$ are related by $\{c_\alpha^\dagger c_\beta^\dagger|0\rangle\} = -\{c_\beta^\dagger c_\alpha^\dagger|0\rangle\}$. One thus gets,

$$|n_2\rangle = \sum_{\alpha<\beta} X(\alpha\beta; n_2) c_\alpha^\dagger c_\beta^\dagger|0\rangle \tag{16}$$

The TDA eigenvectors $\langle n_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle$ and the wave function amplitudes X are related by,

$$\langle m_2|n_2\rangle = \delta_{m_2 n_2} = \sum_{\alpha<\beta} X(\alpha\beta; n_2)\langle m_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle$$

since the basis states $c_\alpha^\dagger c_\beta^\dagger|0\rangle$ form an independent set of unit vectors, it should be $X(\alpha\beta; n_2) = \langle n_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle^*$