KTH ROYAL INSTITUTE
OF TECHNOLOGY

Second Quantization

April 21, 2017

Creation and annihilation operators. Occupation number. Anticonmutation relations. **Normal product. Wick's theorem.** One-body operator in second quantization. Hartree-Fock potential. Two-particle Random Phase Approximation (RPA). Two- particle Tamm-Damkoff Approximation (TDA).

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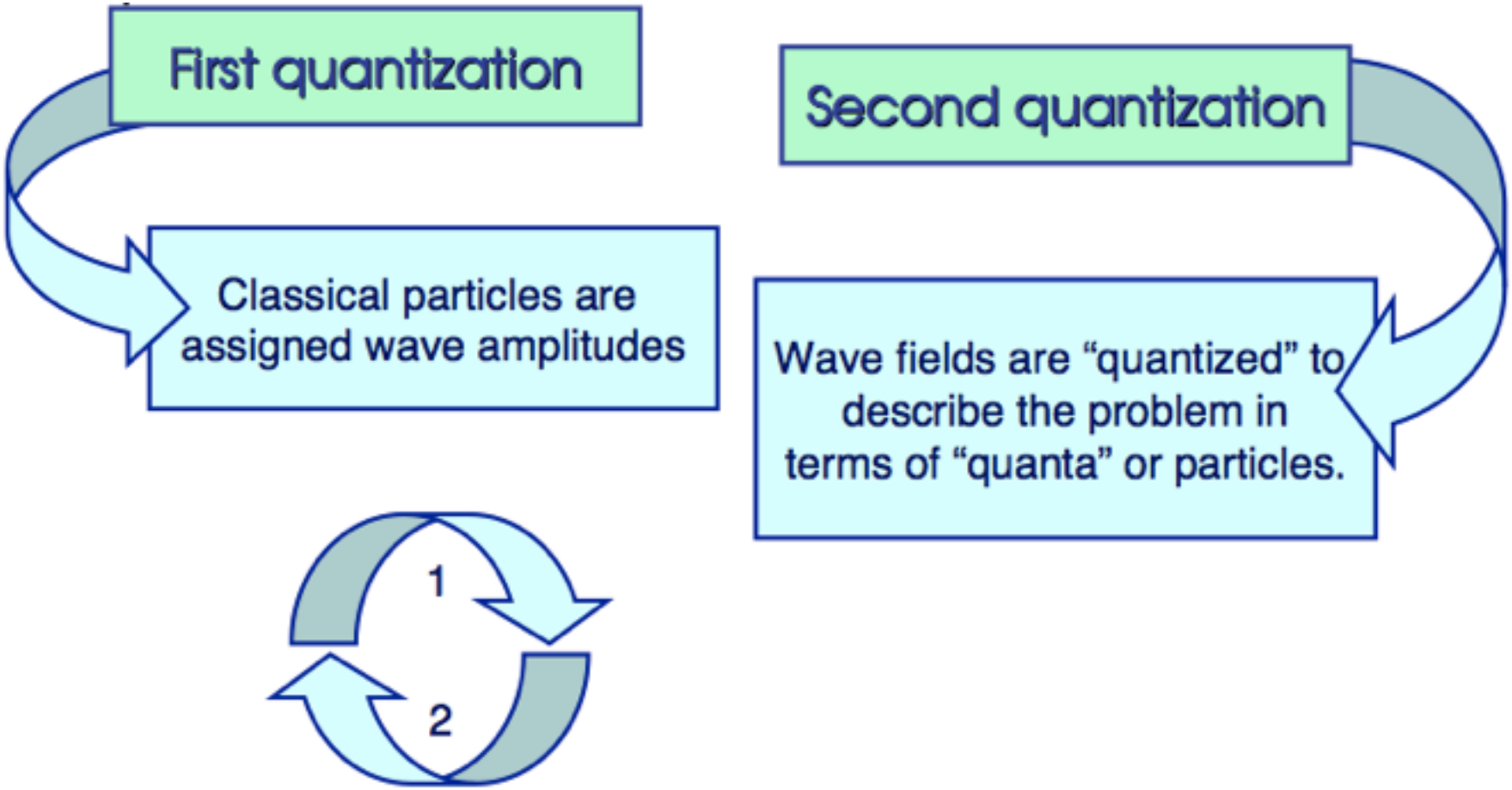
First & second quantizations



Simple Harmonic Oscillator

$$H = \frac{1}{2}\frac{p^2}{m} - \frac{1}{2}m\omega^2 x^2$$

A more general solution is

$$x(t) = c_1 e^{i\omega t} + c_2 e^{-i\omega t}$$

To quantize it, we say

$$[x, p] = i\hbar$$

A very very important trick is to write this as

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

with

$$[a, a^\dagger] = 1$$

Then

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$$

Thus energy eigenstates are eigenstates of the number operator

$$N = a^\dagger a$$

In Second Quantization one introduces the creation operator such that a state can be written as

$$|p_i\rangle = c^\dagger_{p_i}|0\rangle$$

this state has to be normalized, that is,

$$\langle p_i|p_i\rangle = \langle 0|c_{p_i}c^\dagger_{p_i}|0\rangle = \langle 0|c_{p_i}|p_i\rangle = 1$$

from where it follows that

$$|0\rangle = c_{p_i}|p_i\rangle$$

and the operator c_{p_i} can be interpreted as the annihilation operator of a particle

Vacuum

$$\langle 0|0\rangle = 1$$

$$a_k|0\rangle = 0$$

$$\langle 0|a^\dagger_k = 0$$

There is no particle to annihilation in “vacuum”

$$N|n\rangle = n|n\rangle$$

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

$$a|n\rangle = \sqrt{n}|n-1\rangle$$

Reminder, for boson $[a, a^\dagger] = 1$

Anticommutation relation

The operation

$$\{A, B\} = AB + BA$$

is called the anticommutator of A and B, and these operators anticommute if

$$\{A, B\} = 0$$

Summing these two equations one gets,

$$\langle 0|c_k c_j^\dagger + c_j^\dagger c_k|0\rangle = \delta_{jk}$$

which is valid independently of whether $|j\rangle$ and $|k\rangle$ are particle or hole states. It is a general equation and, therefore, the creation-annihilation operators satisfy

$$\{c_j, c_k^\dagger\} = \delta_{jk}.$$

Reminder, for boson $[a, a^\dagger] = 1$

$$\left\{a_i^\dagger, a_j^\dagger\right\} = a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = 0$$

$$\left\{a_i, a_j\right\} = a_i a_j + a_j a_i = 0$$

$$\left\{a_i, a_j^\dagger\right\} = a_i a_j^\dagger + a_j^\dagger a_i = \delta_{ij}$$

Hole state

Below the Fermi level (FL) all states are occupied and one can not place a particle there. In other words, the A-particle state $|0\rangle$, with all levels hi occupied, is the ground state of the inert (frozen) double magic core.

This implies that the hole state h_i in the (A-1)-nucleon system is

$$|h_i\rangle = c_{h_i}|0\rangle$$

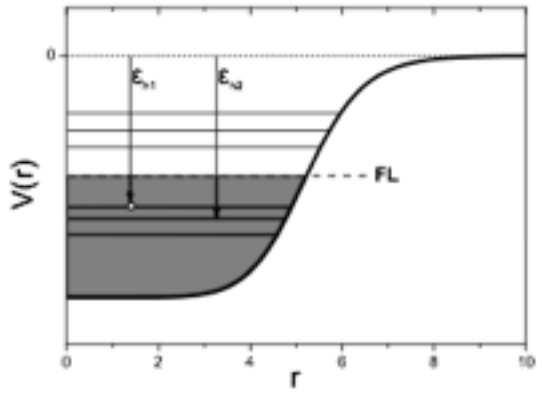


Figure 5: Excitations h_i in the (A-1)-particle nucleus. It looks like at the level h_1 there is a hole in the completely filled states of the core. Therefore the states below the Fermi level are called "hole excitations". A hole at the more deeply bound level h_2 induces a higher excitation than the one at h_1.

Occupation number

One notices that the number

$$n_j = \langle 0|c_j^\dagger c_j|0\rangle$$

is $n_j = 1$ is j is a hole state and $n_j = 0$ if j is a particle state. In the same fashion it is $\langle 0|c_j c_j^\dagger|0\rangle = 1$ (0) if j is a particle (hole) state, that is $\langle 0|c_j c_j^\dagger|0\rangle = 1$ - n_j. Therefore n_j is called occupation number of the state j.

In general it is

$$\langle 0|c_j^\dagger c_k|0\rangle = n_j \delta_{jk},$$

and

$$\langle 0|c_k c_j^\dagger|0\rangle = (1 - n_j)\delta_{jk}.$$

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$$

Thus energy eigenstates are eigenstates of the number operator

$$N = a^\dagger a$$

which is Hermetian. Also, all the stuff we saw last time is true

$$N|n\rangle = n|n\rangle$$

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

$$a|n\rangle = \sqrt{n}|n-1\rangle$$

First quantizaiton:
Slater determinant

Second quantizaiton

$$\Psi_{jk}(q_1,q_2) = \frac{1}{\sqrt{2}}\begin{vmatrix}\psi_j(q_1) & \psi_k(q_2)\\ \psi_j(q_2) & \psi_k(q_2)\end{vmatrix} \Rightarrow |jk\rangle = a_j^\dagger a_k^\dagger |0\rangle$$

States

$a_i^\dagger|0\rangle$ one-particle state

$a_i^\dagger a_j^\dagger|0\rangle$ two-particle state

$a_i^\dagger a_j^\dagger \ldots a_n^\dagger|0\rangle$ N-particle state

} described by Slater determinants in first quantization

$$|a \otimes b\rangle_B = \frac{1}{\sqrt{2}}\left(|a_1 \otimes b_2\rangle + |a_2 \otimes b_1\rangle\right) \qquad \text{bosons; symmetric}$$

$$|a \otimes b\rangle_F = \frac{1}{\sqrt{2}}\left(|a_1 \otimes b_2\rangle - |a_2 \otimes b_1\rangle\right) \qquad \text{fermions; anti} - \text{symmetric}$$

◇Convenient to describe processes in which particles are created and annihilated;
◇Convenient to describe interactions.

First quantizaiton: Slater determinant

Second quantizaiton

$$\Psi_{jk}(q_1, q_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \psi_j(q_1) & \psi_k(q_2) \\ \psi_j(q_2) & \psi_k(q_2) \end{vmatrix} \Rightarrow |jk\rangle = a_j^\dagger a_k^\dagger |0\rangle$$

In second quantization the antisymmetrized two-particle state is $|ij\rangle_a = c_i^\dagger c_j^\dagger |0\rangle$, since it implies

$$c_i^\dagger c_j^\dagger = -c_j^\dagger c_i^\dagger \Longrightarrow c_i^\dagger c_i^\dagger = 0$$

as required by the Pauli principle. In the same fashion

$$c_i c_j = -c_j c_i$$

Therefore

$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0$$

Since the state $|0\rangle$ corresponds to a nucleus with $A = N + Z$ nucleons, the state $c_i^\dagger c_j^\dagger |0\rangle$ corresponds to $A + 2$ nucleons. Therefore

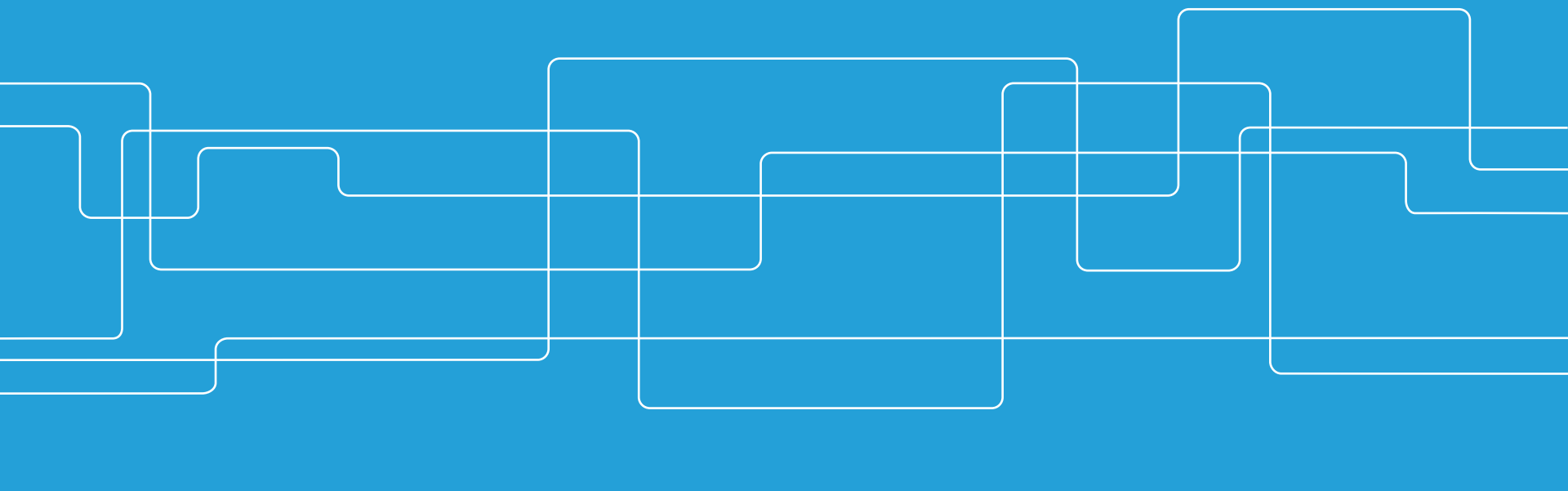
$$\langle 0|c_i^\dagger c_j^\dagger|0\rangle = 0, \quad \langle 0|c_i c_j|0\rangle = 0$$

for all i and j.

Normal product

Operators in second quantization
Creation/Annihilation operations

April 27, 2016



Occupation Number Formalism

Fermion Creation and Annihilation Operators

$$c_i \left| n_1 n_2 \ldots n_i \ldots \right\rangle = (-1)^{\sum_i} \; n_i \left| n_1 n_2 \ldots n_{i-1} \ldots \right\rangle$$

$$c_i^+ \left| n_1 n_2 \ldots n_i \ldots \right\rangle = (-1)^{\sum_i} \; (1 - n_i) \left| n_1 n_2 \ldots n_{i+1} \ldots \right\rangle$$

$\sum_i = n_1 + n_2 + \ldots + n_{i-1}$ i.e. number of particles to left of ith

Boson Creation and Annihilation Operators

$$a_i \left| n_1 n_2 \ldots n_i \ldots \right\rangle = n_i^{1/2} \left| n_1 n_2 \ldots n_i \ldots \right\rangle$$

$$a_i^+ \left| n_1 n_2 \ldots n_i \ldots \right\rangle = (n_i + 1)^{1/2} \left| n_1 n_2 \ldots n_i \ldots \right\rangle$$

Fermion examples

$$c_3 \left| 1111100 \right\rangle = (-1)^{1+1} 1 \left| 1101100 \right\rangle = \left| 1101100 \right\rangle$$

$$c_4^+ \left| 1110110 \right\rangle = (-1)^{1+1+1} 1 \left| 1111110 \right\rangle = - \left| 1111110 \right\rangle$$

Occupation number

One notices that the number

$$n_j = \langle 0|c_j^\dagger c_j|0\rangle$$

is $n_j = 1$ is j is a hole state and $n_j = 0$ if j is a particle state. In the same fashion it is $\langle 0|c_j c_j^\dagger|0\rangle = 1$ (0) if j is a particle (hole) state, that is $\langle 0|c_j c_j^\dagger|0\rangle = 1$ - n_j. Therefore n_j is called occupation number of the state j.

In general it is

$$\langle 0|c_j^\dagger c_k|0\rangle = n_j \delta_{jk},$$

and

$$\langle 0|c_k c_j^\dagger|0\rangle = (1 - n_j)\delta_{jk}.$$

Normal product (order)

Normal ordering for fermions is defined by rearranging all creation operators to the left of annihilation operators, but keeping track of the anti-commutations relations at each operator exchange.

Normal product (order)

Since $\langle 0|c_i c_j^\dagger|0\rangle = (1-n_i)\delta_{ij}$, one can write

$$c_i c_j^\dagger = (1-n_i)\delta_{ij} + : c_i c_j^\dagger :$$

where $: c_i c_j^\dagger :$ is defined by the relation,

$$\langle 0| : c_i c_j^\dagger : |0\rangle = 0$$

The operator $: AB :$ is called normal product between A and B. In the same fashion

$$c_i^\dagger c_j = n_i \delta_{ij} + : c_i^\dagger c_j :$$

From these equations one gets (using $\{c_i, c_j^\dagger\} = \delta_{ij}$)

$$c_j c_i^\dagger = \delta_{ij} - c_i^\dagger c_j = (1-n_i)\delta_{ij} - : c_i^\dagger c_j :$$

but

$$c_j c_i^\dagger = (1-n_i)\delta_{ij} + : c_j c_i^\dagger :$$

$$: c_j c_i^\dagger := - : c_i^\dagger c_j :$$

Contraction

One uses the notation

$$\overbrace{c_i c_j^\dagger} = (1 - n_i)\delta_{ij}; \quad \overbrace{c_i^\dagger c_j} = n_i \delta_{ij}$$

The operation $\overbrace{AB}$ is called contraction of the operators A and B. The contraction is a number.

The contraction of arbitrary creation or annihilation operators A and B designated by

$$\overbrace{A\,B}$$

is defined as the difference between the ordinary and the normal product of the operators A and B :

$$\overbrace{A\,B} = AB - :AB:$$

Already in normal form

$$a_i^\dagger a_j^\dagger =: a_i^\dagger a_j^\dagger : \;\rightarrow\; \overbrace{a_i^\dagger a_j^\dagger} = 0$$

$$a_i a_j =: a_i a_j : \;\rightarrow\; \overbrace{a_i a_j} = 0$$

We defined

$$c_i^\dagger c_j = n_i \delta_{ij} + : c_i^\dagger c_j :$$

$$\overbrace{c_i c_j^\dagger} = (1 - n_i)\delta_{ij}; \quad \overbrace{c_i^\dagger c_j} = n_i \delta_{ij}$$

Thus

$$c_i^\dagger c_j = \overbrace{c_i^\dagger c_j} + : c_i^\dagger c_j :$$

Wick's theorem

The next degree of complication is when two contractions are possible, for instance

$$
\begin{aligned}
c_i^\dagger c_j c_k c_l^\dagger = &: c_i^\dagger c_j c_k c_l^\dagger : \\
&+ \overbrace{c_i^\dagger c_j} : c_k c_l^\dagger : - \overbrace{c_i^\dagger c_k} : c_j c_l^\dagger : - \overbrace{c_j c_l^\dagger} : c_i^\dagger c_k : + \overbrace{c_k c_l^\dagger} : c_i^\dagger c_j : \\
&+ \overbrace{c_i^\dagger c_j}\, \overbrace{c_k c_l^\dagger} - \overbrace{c_i^\dagger c_k}\, \overbrace{c_j c_l^\dagger}
\end{aligned}
$$

one needs one permutation to get the term $\overbrace{c_i^\dagger c_k} : c_j c_l^\dagger$ and therefore a minus sign is added. The same is done to get the signs of all other terms. The mean value of this operator is,

$$
\langle 0 | c_i^\dagger c_j c_k c_l^\dagger | 0 \rangle = \overbrace{c_i^\dagger c_j}\, \overbrace{c_k c_l^\dagger} - \overbrace{c_i^\dagger c_k}\, \overbrace{c_j c_l^\dagger} = n_i \delta_{ij} (1 - n_k) \delta_{kl} - n_i \delta_{ik} (1 - n_j) \delta_{jl}
$$

Wick's theorem

One can write any product of creation and annihilation operators in normal form by using the Wick's Theorem. It says that the product of operators,

$$A_1 A_2 A_3 \cdots A_{n-1} A_n$$

where A_i is $c_i^\dagger$ or c_i, can be written as

$$\begin{aligned} A_1 A_2 A_3 \cdots A_{n-1} A_n = &: A_1 A_2 A_3 \cdots A_{n-1} A_n : \\ &+ \overbrace{A_1 A_2} : A_3 \cdots A_{n-1} A_n : \\ &- \overbrace{A_1 A_3} : A_2 \cdots A_{n-1} A_n : \\ &+ \cdots \text{ (all single-contractions)} \\ &+ \overbrace{A_1 A_2}\, \overbrace{A_3 A_4} : A_5 \cdots A_{n-1} A_n : \\ &- \overbrace{A_1 A_3}\, \overbrace{A_2 A_4} : A_5 \cdots A_{n-1} A_n : \\ &+ \cdots \text{ (all double-contractions)} \\ &+ \cdots \text{ (upto } n/2\text{-contractions)} \end{aligned}$$

The plus or minus sign in each term is determined by the number of permutations one must do in order to arrive to the final form of the term. An odd (even) number of permutation gives a minus (plus) sign.

The great property of this theorem is that it allows one to get in a straightforward fashion the mean value of the product of operators, which is what one usually needs. This number is just the term without normal products, i. e. the last two terms in the equation above.

Every operator in the Fock's space can be written as a product of creation and annihilation operators. In general, every operation takes the form:

$$\sum_{mn=0}^{M} \hat{O}(m,n),$$

m creation and n annihilation operators in normal order

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,

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

II

Random Phase approximation and Tamm-Dancoff approximation

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,

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

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

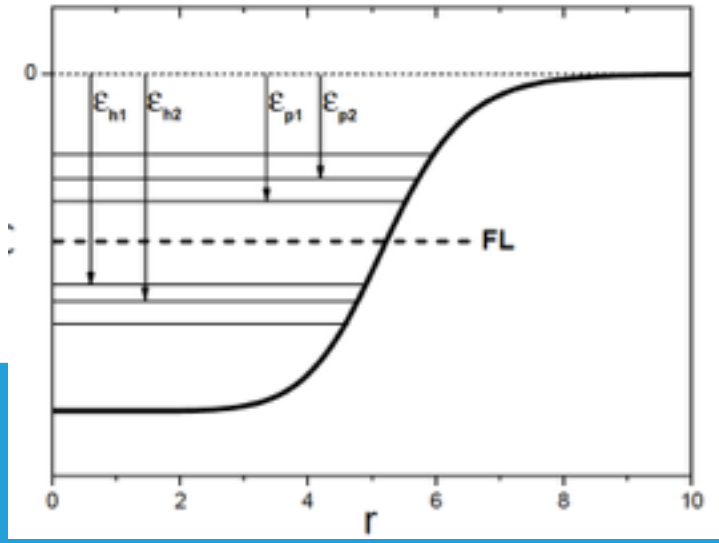
$$H_{HF} = \sum_{\alpha\beta}\left(\langle\alpha|T|\beta\rangle + \sum_\gamma n_\gamma \langle\alpha\gamma|V|\beta\gamma\rangle_a\right) : c_\alpha^\dagger c_\beta :$$

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

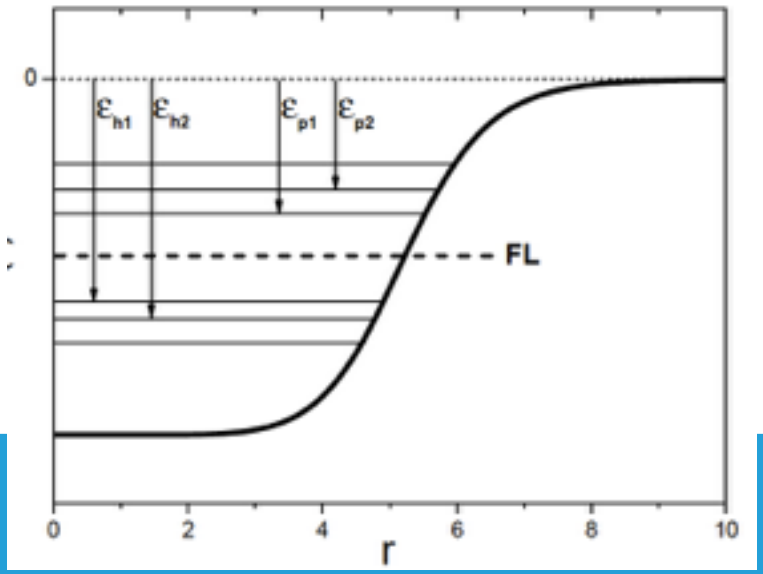
$$\langle j|H_{HF}|i\rangle = \varepsilon_i \delta_{ij}$$

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.

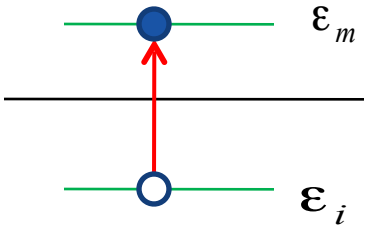
Closed shell: 1p-1h correlation

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

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

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

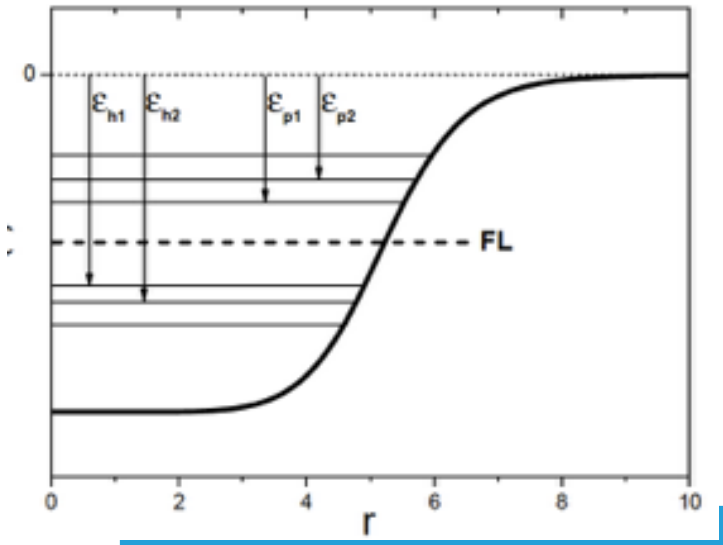
$$B_{mi\,nj} = \tilde{v}_{mnij}$$

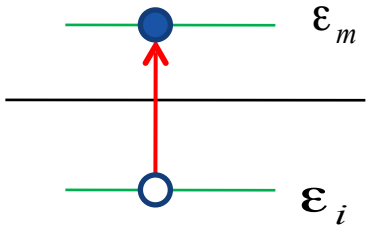
Tamm-Damkoff Approximation (TDA)

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-Dankoff 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 $X(\alpha\beta; n_2) = \langle n_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle^*$