Chapter 7

Second Quantization

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

7.1 Creation and annihilation operators

In Fig. 3 of the previous Chapter it is shown the single-particle levels generated by a double-magic core containing A nucleons. Below the Fermi level (FL) all states h_i are occupied and one can not place a particle there. In other words, the A-particle state $|0\rangle$, with all levels h_i occupied, is the ground state of the inert (frozen) double magic core.

Above the FL all states are empty and, therefore, a particle can be created in one of the levels denoted by p_i in the Figure. In Second Quantization one introduces the creation operator $c^\dagger_{p_i}$ such that the state $|p_i\rangle$ in the nucleus containing A+1 nucleons can be written as,

$$|p_i\rangle = c^\dagger_{p_i}|0\rangle \tag{7.1}$$

this state has to be normalized, that is,

$$\langle p_i|p_i\rangle = \langle 0|c_{p_i}c^\dagger_{p_i}|0\rangle = \langle 0|c_{p_i}|p_i\rangle = 1 \tag{7.2}$$

from where it follows that

$$|0\rangle = c_{p_i}|p_i\rangle \tag{7.3}$$

and the operator c_{p_i} can be interpreted as the annihilation operator of a particle in the state $|p_i\rangle$. This implies that the hole state h_i in the (A-1)-nucleon system is

$$|h_i\rangle = c_{h_i}|0\rangle \tag{7.4}$$

Occupation number and anticommutation relations

One notices that the number

$$n_j = \langle 0|c^\dagger_j c_j|0\rangle \tag{7.5}$$

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 $\langle 0|c_j c^\dagger_j|0\rangle = 1$ (0) if j is a particle (hole) state, that is $\langle 0|c_j c^\dagger_j|0\rangle = 1$ - n_j. Therefore n_j is called occupation number of the state j.

In general it is

$$\langle 0|c^\dagger_j c_k|0\rangle = n_j\delta_{jk}, \tag{7.6}$$

and

$$\langle 0|c_k c_j^\dagger|0\rangle = (1 - n_j)\delta_{jk}. \tag{7.7}$$

Summing these two equations one gets,

$$\langle 0|c_k c_j^\dagger + c_j^\dagger c_k|0\rangle = \delta_{jk} \tag{7.8}$$

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

$$\{c_j, c_k^\dagger\} = \delta_{jk}. \tag{7.9}$$

The operation

$$\{A, B\} = AB + BA \tag{7.10}$$

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

$$\{A, B\} = 0 \tag{7.11}$$

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

$$c_i^\dagger c_j^\dagger = -c_j^\dagger c_i^\dagger \Longrightarrow c_i^\dagger c_i^\dagger = 0 \tag{7.12}$$

as required by the Pauli principle. In the same fashion

$$c_i c_j = -c_j c_i \tag{7.13}$$

Therefore

$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0 \tag{7.14}$$

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

$$\langle 0|c_i^\dagger c_j^\dagger|0\rangle = 0, \quad \langle 0|c_i c_j|0\rangle = 0 \tag{7.15}$$

for all i and j.

7.2 Normal product

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

$$c_i c_j^\dagger = (1 - n_i)\delta_{ij} + : c_i c_j^\dagger : \tag{7.16}$$

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

$$\langle 0| : c_i c_j^\dagger : |0\rangle = 0 \tag{7.17}$$

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

$$c_i^\dagger c_j = n_i \delta_{ij} + : c_i^\dagger c_j : \tag{7.18}$$

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

$$c_j c_i^\dagger = \delta_{ij} - c_i^\dagger c_j = (1 - n_i)\delta_{ij} - : c_i^\dagger c_j : \tag{7.19}$$

but

$$c_j c_i^\dagger = (1 - n_i)\delta_{ij} + : c_j c_i^\dagger : \tag{7.20}$$

$$: c_j c_i^\dagger := - : c_i^\dagger c_j : \tag{7.21}$$

One uses the notation

$$\overbrace{c_i c_j^\dagger} = (1 - n_i)\delta_{ij}; \quad \overbrace{c_i^\dagger c_j} = n_i \delta_{ij} \tag{7.22}$$

The operation $\overbrace{AB}$ is called contraction of the operators A and B. The contraction is a number. It is defined as the difference between the ordinary and the normal product of the operators A and B.

Therefore,

$$\overbrace{c_i^\dagger c_j^\dagger} = \overbrace{c_i c_j} = 0 \tag{7.23}$$

from where one gets,

$$c_i^\dagger c_j^\dagger =: c_i^\dagger c_j^\dagger :, \quad c_i c_j =: c_i c_j : \tag{7.24}$$

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,

$$A_1 A_2 A_3 \cdots A_{n-1} A_n \tag{7.25}$$

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

$$\begin{aligned} A_1 A_2 A_3 \cdots A_{n-1} A_n = & : A_1 A_2 A_3 \cdots A_{n-1} A_n : \\ & + \overbrace{A_1 A_2} : A_3 \cdots A_{n-1} A_n : \\ & - \overbrace{A_1 A_3} : A_2 \cdots A_{n-1} A_n : \\ & + \cdots \text{ (all single-contractions)} \\ & + \overbrace{A_1 A_2}\,\overbrace{A_3 A_4} : A_5 \cdots A_{n-1} A_n : \\ & - \overbrace{A_1 A_3}\,\overbrace{A_2 A_4} : A_5 \cdots A_{n-1} A_n : \\ & + \cdots \text{ (all double-contractions)} \\ & + \cdots \text{ (upto } n/2\text{-contractions)} \end{aligned} \tag{7.26}$$

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 term in the equation above.

We have

$$\begin{aligned}\langle 0|:A_1A_2A_3\cdots A_{n-1}A_n:|0\rangle =&\langle 0|A_1A_2A_3\cdots A_{n-1}A_n|0\rangle \\ &-\langle 0|A_1A_2A_3\cdots A_{n-1}A_n|0\rangle\langle 0|0\rangle \\ =&0\end{aligned} \tag{7.27}$$

The "normal product" of a normal product

$$::AB::=\overbrace{:AB:}+::AB::=:AB: \tag{7.28}$$

The best way of understanding how this theorem works is by applying it to simple cases, We start by the product

$$c_i^\dagger c_j=\overbrace{c_i^\dagger c_j}+:c_i^\dagger c_j: \tag{7.29}$$

where only one contraction is possible and no permutation is needed to reach the final value, that is the sign is plus. As expected, one gets, $\langle 0|c_i^\dagger c_j|0\rangle=\overbrace{c_i^\dagger c_j}$

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

$$\begin{aligned}c_i^\dagger c_jc_kc_l^\dagger =&:c_i^\dagger c_jc_kc_l^\dagger : \\ &+\overbrace{c_i^\dagger c_j}:c_kc_l^\dagger :-\overbrace{c_i^\dagger c_k}:c_jc_l^\dagger :-\overbrace{c_jc_l^\dagger}:c_i^\dagger c_k:+\overbrace{c_kc_l^\dagger}:c_i^\dagger c_j: \\ &+\overbrace{c_i^\dagger c_j}\,\overbrace{c_kc_l^\dagger}-\overbrace{c_i^\dagger c_k}\,\overbrace{c_jc_l^\dagger}\end{aligned} \tag{7.30}$$

one needs one permutation to get the term $\overbrace{c_i^\dagger c_k}:c_jc_l^\dagger$ 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,

$$\langle 0|c_i^\dagger c_jc_kc_l^\dagger|0\rangle=\overbrace{c_i^\dagger c_j}\,\overbrace{c_kc_l^\dagger}-\overbrace{c_i^\dagger c_k}\,\overbrace{c_jc_l^\dagger}=n_i\delta_{ij}(1-n_k)\delta_{kl}-n_i\delta_{ik}(1-n_j)\delta_{jl} \tag{7.31}$$

Further examples

We have

$$\begin{aligned}:c_i^\dagger c_i:c_\alpha^\dagger c_\beta^\dagger =&+\overbrace{c_ic_\alpha^\dagger}:c_i^\dagger c_\beta^\dagger :-\overbrace{c_ic_\beta^\dagger}:c_i^\dagger c_\alpha^\dagger : \\ &+:c_i^\dagger c_ic_\alpha^\dagger c_\beta^\dagger :,\end{aligned} \tag{7.32}$$

and

$$\begin{aligned}c_\alpha^\dagger c_\beta^\dagger :c_i^\dagger c_i:=&-\overbrace{c_\alpha^\dagger c_i}:c_i^\dagger c_\beta^\dagger :+\overbrace{c_\beta^\dagger c_i}:c_i^\dagger c_\alpha^\dagger : \\ &+:c_\alpha^\dagger c_\beta^\dagger c_i^\dagger c_i:,\end{aligned} \tag{7.33}$$

from which we get

$$[:c_i^\dagger c_i:,c_\alpha^\dagger c_\beta^\dagger]=\delta_{i\alpha}:c_i^\dagger c_\beta^\dagger :-\delta_{i\beta}:c_i^\dagger c_\alpha^\dagger :. \tag{7.34}$$

We also have

$$\begin{aligned}:c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta :c_i^\dagger c_j^\dagger =&:c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta c_i^\dagger c_j^\dagger : \\ &-\overbrace{c_\gamma c_i^\dagger}:c_\alpha^\dagger c_\beta^\dagger c_\delta c_j^\dagger :+\cdots\ \text{(other three single contractions)} \\ &-\overbrace{c_\gamma c_i^\dagger}\,\overbrace{c_\delta c_j^\dagger}:c_\alpha^\dagger c_\beta^\dagger :+\overbrace{c_\gamma c_j^\dagger}\,\overbrace{c_\delta c_i^\dagger}:c_\alpha^\dagger c_\beta^\dagger :\end{aligned} \tag{7.35}$$

and one finds, after some algebra

$$\begin{aligned}[: c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta :, c_i^\dagger c_j^\dagger] = &- \delta_{\gamma i} : c_\alpha^\dagger c_\beta^\dagger c_\delta c_j^\dagger : + \cdots \text{ (other three single contractions)} \\ &+ (1 - n_i - n_j)(-\delta_{\gamma i}\delta_{\delta j} + \delta_{\gamma i}\delta_{\delta j}) : c_\alpha^\dagger c_\beta^\dagger :\end{aligned} \tag{7.36}$$

7.3 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,

$$\hat{M} = \sum_{pq} \langle p|\hat{M}|q\rangle c_p^\dagger c_q = \sum_{pq} \langle p|\hat{M}|q\rangle [: c_p^\dagger c_q : + \overbrace{c_p^\dagger c_q}] \tag{7.37}$$

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 should be that we get the matrix element itself again.

We then evaluate

$$\begin{aligned}\langle i|\hat{M}|j\rangle =& \langle 0|c_i \hat{M} c_j^\dagger|0\rangle = \sum_{pq} \langle p|\hat{M}|q\rangle \langle 0|c_i c_p^\dagger c_q c_j^\dagger|0\rangle \\ =& \sum_{pq} \langle p|\hat{M}|q\rangle \langle 0|\overbrace{c_i c_p^\dagger}\overbrace{c_q c_j^\dagger} + \overbrace{c_i c_j^\dagger}\overbrace{c_p^\dagger c_q}|0\rangle \\ =& \sum_{pq} \langle p|\hat{M}|q\rangle \Big[(1-n_i)\delta_{ip}(1-n_j)\delta_{qj} + (1-n_i)\delta_{ij}n_p\delta_{pq}\Big] \\ =& (1-n_i)(1-n_j)\langle i|\hat{M}|j\rangle + (1-n_i)\delta_{ij}\sum_p n_p \langle p|\hat{M}|p\rangle\end{aligned} \tag{7.38}$$

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

$$\hat{M} = \sum_{pq} \langle p|\hat{M}|q\rangle : c_p^\dagger c_q : \tag{7.39}$$

that is, one assumes that $\hat{M}$ itself includes polarization. One sees that this avoids the core polarization term, since one cannot contract the indexes p and q (i. e. the term δ_{pq} in Eq. (7.38)). Therefore the core polarization effects were assumed to be contained in the operator itself. This procedure is called "renormalization". It is done by introducing some parameters that takes proper account of the polarization. We will see that in electromagnetic transitions this is done by defining an effective charge for protons and also for neutrons which, without polarization, has no charge at all.

7.4 Two-body operator in second quantization

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,

$$\hat{M} = \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta|\hat{M}|\gamma\delta\rangle : c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma : \tag{7.40}$$

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 it is worthwhile to point out that a great advantage of second quantization is that in the many-particle case the Pauli principle is automatically taken into account.

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,

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

which give,

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

In r-representation the matrix element is

$$\langle ij|\hat{M}|kl\rangle = \int \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \big(\Psi_i(\boldsymbol{r}_1)\Psi_j(\boldsymbol{r}_2)\big)^* \hat{M}(\boldsymbol{r}_1,\boldsymbol{r}_2)\Psi_k(\boldsymbol{r}_1)\Psi_l(\boldsymbol{r}_2) \tag{7.45}$$

and due to the principle of action and reaction it is, $\hat{M}(\boldsymbol{r}_1,\boldsymbol{r}_2) = \hat{M}(\boldsymbol{r}_2,\boldsymbol{r}_1)$ which, according to Eq. (7.45), implies $\langle ij|\hat{M}|kl\rangle = \langle ji|\hat{M}|lk\rangle$.

The matrix element antisymmetrized to the right only becomes,

$$\langle ji|\hat{M}|kl\rangle_a = \langle ji|\hat{M}\big[|kl\rangle - |lk\rangle\big] = \langle ij|\hat{M}\big[|lk\rangle - |kl\rangle\big] = -\langle ij|\hat{M}|kl\rangle_a \tag{7.46}$$

and Eq. (7.44) becomes,

$${}_a\langle ij|\hat{M}|kl\rangle_a = (1-n_i)(1-n_j)(1-n_k)(1-n_l)\,{}_a\langle ij|\hat{M}|kl\rangle_a \tag{7.47}$$

which is just what we wanted to show. However, one does not need to take the matrix element with antisymmetric wave functions in bra as well as in ket positions since ${}_a\langle ij|\hat{M}|kl\rangle_a = 2\langle ij|\hat{M}|kl\rangle_a$. Therefore to obtain the matrix element $\langle ij|\hat{M}|kl\rangle_a$ one has to add a factor 1/4 to the expression (7.40), i. e.

$$\hat{M} = \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{M}|\gamma\delta\rangle : c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma : \tag{7.48}$$

This is the expression that is used in general. We will use it here also.

7.5 Hartree-Fock potential

We found that to avoid core excitations the one-body operator should be defined in terms of normal products. That is to use $: c_\alpha^\dagger c_\beta :$ instead of $c_\alpha^\dagger c_\beta$. 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 physics behind the core excitations in the case of two-body operators, particularly in the Hamiltonian. This is what we will explore now.

To this end we write the Hamiltonian $H = T + V$ in a representation consisting of the eigenvectors of another Hamiltonian. This is often chosen to be an Harmonic oscillator representation because it is mathematically easy to deal with and also because the nuclear bound states are well described by Harmonic oscillator potentials, as we have seen in the previous Chapter. Within the chosen representation (labeled by Greek letters below) the Hamiltonian becomes,

$$H = \sum_{\alpha\beta}\langle\alpha|T|\beta\rangle c_\alpha^\dagger c_\beta + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\gamma\delta\rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma. \tag{7.49}$$

Converting to normal form one gets,

$$\begin{aligned} H = &\sum_{\alpha\beta}\langle\alpha|T|\beta\rangle(: c_\alpha^\dagger c_\beta : + \overbrace{c_\alpha^\dagger c_\beta}) + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\gamma\delta\rangle[: c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma : \\ &+ : c_\alpha^\dagger c_\gamma : \overbrace{c_\beta^\dagger c_\delta} - : c_\alpha^\dagger c_\delta : \overbrace{c_\beta^\dagger c_\gamma} - : c_\beta^\dagger c_\gamma : \overbrace{c_\alpha^\dagger c_\delta} + : c_\beta^\dagger c_\delta : \overbrace{c_\alpha^\dagger c_\gamma} \\ &+ \overbrace{c_\alpha^\dagger c_\gamma}\,\overbrace{c_\beta^\dagger c_\delta} - \overbrace{c_\alpha^\dagger c_\delta}\,\overbrace{c_\beta^\dagger c_\gamma}], \end{aligned} \tag{7.50}$$

where, as was shown before, we have $\overbrace{c_i c_j^\dagger} = (1 - n_i)\delta_{ij}$ and $\overbrace{c_i^\dagger c_j} = n_i\delta_{ij}$. After some algebra to be performed,

$$H = E_0 + H_{HF} + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\gamma\delta\rangle : c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma : \tag{7.51}$$

where

$$E_0 = \sum_\alpha n_\alpha\langle\alpha|T|\alpha\rangle + \frac{1}{2}\sum_{\alpha\beta} n_\alpha n_\beta\langle\alpha\beta|V|\alpha\beta\rangle_a \tag{7.52}$$

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

$$H_{HF} = \sum_{\alpha\beta} \left(\langle \alpha|T|\beta\rangle + \sum_{\gamma} n_\gamma \langle \alpha\gamma|V|\beta\gamma\rangle_a \right) : c^\dagger_\alpha c_\beta : \tag{7.53}$$

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.

$$H_{HF} = \sum_{\alpha\beta} |\alpha\rangle \left(\langle \alpha|T|\beta\rangle + \sum_{\gamma} n_\gamma \langle \alpha\gamma|V|\beta\gamma\rangle_a \right) \langle\beta| \tag{7.54}$$

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

$$H_{HF}|i\rangle = \varepsilon_i |i\rangle \tag{7.55}$$

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

$$\sum_{\beta} \left(\langle \alpha|T|\beta\rangle + \sum_{\gamma} n_\gamma \langle \alpha\gamma|V|\beta\gamma\rangle_a \right) \langle\beta|i\rangle = \varepsilon_i \langle\alpha|i\rangle \tag{7.56}$$

and the eigenvectors are obtained by imposing the normalization condition,

$$|i\rangle = \sum_{\alpha} \langle\alpha|i\rangle |\alpha\rangle, \quad \langle i|i\rangle = 1 \tag{7.57}$$

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

$$\langle j|H_{HF}|i\rangle = \varepsilon_i \delta_{ij} \tag{7.58}$$

If it is not then one uses as representation these vectors $\{|i\rangle\}$ (instead of the one labeled by Greek letters) to obtained new eigenvectors, which we call $\{|i'\rangle\}$, satisfying

$$H_{HF}|i'\rangle = \varepsilon_{i'}|i'\rangle, \quad |i'\rangle = \sum_{i} \langle i|i'\rangle |i\rangle \tag{7.59}$$

If the condition $\langle j'|H_{HF}|i'\rangle = \varepsilon'_i \delta_{i'j'}$ is still not fulfilled, then one proceeds as before and chooses $\{|i'\rangle\}$ as representation. One repeats this procedure until one arrives after n attempts, to

$$\langle j^{(n)}|H_{HF}|i^{(n)}\rangle = \varepsilon_{i^{(n)}} \delta_{i^{(n)}j^{(n)}} \tag{7.60}$$

and the states $\{|i^{(n)}\rangle\}$ form the Hartree-Fock representation.

This representation is used very often in shell model studies. It has the advantage of being based in a fully microscopical formalism. This can be contrasted with the one obtained as diagonalization of the shell model potential discussed in the previous Chapter.

7.6 Two-particle 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 subtracted 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,

$$H = \sum_{\alpha} \varepsilon_{\alpha} : c_{\alpha}^{\dagger} c_{\alpha} : + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle : c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma} : \tag{7.61}$$

where ε_{α} is the Hartrre-Fock single-particle energy. The constant energy E_0, Eq. (7.52), is not included because all eigenvalues of the Hamiltonian (7.61) will be referred to the core and, therefore, E_0 plays no role.

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

$$\begin{aligned} \left[H, c_{\alpha}^{\dagger} c_{\beta}^{\dagger} \right] =& \sum_{i} \varepsilon_i \left[: c_i^{\dagger} c_i :, c_{\alpha}^{\dagger} c_{\beta}^{\dagger} \right] + \frac{1}{4} \sum_{ijkl} \langle ij | V | kl \rangle \left[: c_i^{\dagger} c_j^{\dagger} c_l c_k :, c_{\alpha}^{\dagger} c_{\beta}^{\dagger} \right] \\ =& (\varepsilon_{\alpha} + \varepsilon_{\beta}) c_{\alpha}^{\dagger} c_{\beta}^{\dagger} + \frac{1}{2} (1 - n_{\alpha} - n_{\beta}) \sum_{ij} \langle ij | V | \alpha\beta \rangle_a c_i^{\dagger} c_j^{\dagger} \\ & - \frac{1}{2} \sum_{ijl} \langle ij | V | \beta l \rangle_a : c_i^{\dagger} c_j^{\dagger} c_l c_{\alpha}^{\dagger} : + \frac{1}{2} \sum_{ijl} \langle ij | V | \alpha l \rangle_a : c_i^{\dagger} c_j^{\dagger} c_l c_{\beta}^{\dagger} : \end{aligned} \tag{7.62}$$

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 states. With this and noticing that,

$$H|n_2\rangle = E_{n_2} |n_2\rangle, \quad H|0\rangle = E_0 |0\rangle \tag{7.63}$$

one gets,

$$\begin{aligned} \langle n_2 | \left[H, c_{\alpha}^{\dagger} c_{\beta}^{\dagger} \right] | 0 \rangle =& (E_{n_2} - E_0) \langle n_2 | c_{\alpha}^{\dagger} c_{\beta}^{\dagger} | 0 \rangle \\ =& (\varepsilon_{\alpha} + \varepsilon_{\beta}) \langle n_2 | c_{\alpha}^{\dagger} c_{\beta}^{\dagger} | 0 \rangle + (1 - n_{\alpha} - n_{\beta}) \sum_{i<j} \langle ij | V | \alpha\beta \rangle_a \langle n_2 | c_i^{\dagger} c_j^{\dagger} | 0 \rangle \end{aligned} \tag{7.64}$$

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

$$\omega_{n_2} \begin{pmatrix} X_{n_2} \\ Y_{n_2} \end{pmatrix} = \begin{pmatrix} A & B \\ -C & -D \end{pmatrix} \begin{pmatrix} X_{n_2} \\ Y_{n_2} \end{pmatrix} \tag{7.65}$$

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. (7.64). Due to this, the RPA matrix (7.74) is not Hermitian and, therefore, the energies ω_{n_2} can become complex quantities.

Eq. (7.74) can also be written as,

$$\omega_{n_2} \begin{pmatrix} X_{n_2} \\ Y_{n_2} \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} X_{n_2} \\ -Y_{n_2} \end{pmatrix} \tag{7.66}$$

and taking the adjoint of this equation one gets,

$$\omega^*_{n_2}(X^*_{n_2}, Y^*_{n_2}) = (X^*_{n_2}, -Y^*_{n_2}) \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{7.67}$$

where the properties $A^\dagger = A$, $D^\dagger = D$, $C^\dagger = B$ (and, therefore, $C = B^\dagger$) were used.

Multiplying Eq. (7.67) to the right by $\begin{pmatrix} X_{m_2} \\ -Y_{m_2} \end{pmatrix}$ and using Eq. 7.66 one gets,

$$(\omega^*_{n_2} - \omega_{m_2})(X^*_{n_2}, Y^*_{n_2}) \begin{pmatrix} X_{m_2} \\ -Y_{m_2} \end{pmatrix} = 0 \tag{7.68}$$

If $n_2 \neq m_2$ this Equation implies that

$$(X^*_{n_2}, Y^*_{n_2}) \begin{pmatrix} X_{m_2} \\ -Y_{m_2} \end{pmatrix} = 0 \tag{7.69}$$

and normalizing it to unity one gets,

$$\sum_{\alpha\leq\beta} (1 - n_\alpha - n_\beta) \langle n_2|c^\dagger_\alpha c^\dagger_\beta|0\rangle^* \langle m_2|c^\dagger_\alpha c^\dagger_\beta|0\rangle = \delta_{n_2 m_2} \tag{7.70}$$

which defines the RPA scalar product, or metric. In functional analysis it is also called indefinite inner product.

The two-particle state can be written as,

$$|n_2\rangle = \sum_{\alpha\leq\beta} X(\alpha\beta, n_2) c^\dagger_\alpha c^\dagger_\beta |0\rangle \tag{7.71}$$

and multiplying by $\langle m_2|$ one gets

$$\delta_{n_2 m_2} = \sum_{\alpha\leq\beta} X(\alpha\beta, n_2) \langle m_2|c^\dagger_\alpha c^\dagger_\beta|0\rangle \tag{7.72}$$

since the basis elements form an independent set one finds, comparing with Eq. (7.70),

$$X(\alpha\beta, n_2) = (1 - n_\alpha - n_\beta) \langle n_2|c^\dagger_\alpha c^\dagger_\beta|0\rangle^* \tag{7.73}$$

which is the RPA wave function amplitude.

As an example, we evaluate the energy of the a system with one particle orbital (α) and one hole orbital (β). The RPA equation can be written in a 2×2 matrix form as

$$\omega_{n_2} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} A & B \\ -C & -D \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}. \tag{7.74}$$

We have $A = 2\varepsilon_\alpha + \langle\alpha\alpha|V|\alpha\alpha\rangle^{JT}$ where JT denote the spin and isospin of the two particle state. $D = -2\varepsilon_\beta + \langle\beta\beta|V|\beta\beta\rangle^{JT}$. $B = C = \langle\alpha\alpha|V|\beta\beta\rangle^{JT}$. In such a case we get two solutions for the eigen values, $\omega_{n_2} = \frac{A-D}{2} \pm \sqrt{\left(\frac{A-D}{2}\right)^2 + AD - C^2}$, corresponding to the particle-particle and hole-hole excitations respectively. For a system with no particle-hole correlation, we get $\omega_{n_2} = A$ for the two-particle state and $\omega_{n_2} = -D$ for the two-hole state.

7.7 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-Dankoff approximation (TDA).

This approximation implies that the matrices B and C vanish in Eq. (7.74). The particle- and hole-states decoupled and the RPA equation transforms in two TDA equations, one for particle states, i. e.

$$\omega_{n_2} X_{n_2} = A X_{n_2} \tag{7.75}$$

and the other one for hole states,

$$-\omega_{n_2} Y_{n_2} = D Y_{n_2} \tag{7.76}$$

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

We will study these two cases separately starting from Eq. (7.64). For the two-particle case the TDA thus means $n_\alpha = n_\beta = 0$. That is

$$\begin{aligned}\langle n_2|\left[H, c_\alpha^\dagger c_\beta^\dagger\right]|0\rangle =& (E_{n_2} - E_0)\langle n_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle \\ =& (\varepsilon_\alpha + \varepsilon_\beta)\langle n_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle + \sum_{i<j}\langle ij|V|\alpha\beta\rangle_a \langle n_2|c_i^\dagger c_j^\dagger|0\rangle\end{aligned} \tag{7.77}$$

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

The equation for the two-hole states is better obtained starting from the transverse of the RPA operator form, i. e. by performing the operation $\left[H, c_\alpha^\dagger c_\beta^\dagger\right]^\dagger = (Hc_\alpha^\dagger c_\beta^\dagger)^\dagger - (c_\alpha^\dagger c_\beta^\dagger H)^\dagger = c_\beta c_\alpha H - H c_\beta c_\alpha = [H, c_\alpha c_\beta]$ in Eq. (7.62). One thus obtains,

$$[H, c_\alpha c_\beta] = -(\varepsilon_\alpha + \varepsilon_\beta) c_\alpha c_\beta - (1 - n_\alpha - n_\beta)\sum_{i<j}\langle ij|V|\alpha\beta\rangle_a c_i c_j \tag{7.78}$$

where the contribution from three-particle one-hole operators have been neglected. Since the single-particle levels are hole states, one has $(1 - n_\alpha - n_\beta) =$ -1 and the TDA equation for the states $|n_2\rangle$ in the (A-2) nucleus is

$$\begin{aligned}\langle n_2|\left[H, c_\alpha c_\beta\right]|0\rangle =& (E_{n_2} - E_0)\langle n_2|c_\alpha c_\beta|0\rangle \\ =& -(\varepsilon_\alpha + \varepsilon_\beta)\langle n_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle + \sum_{i<j}\langle ij|V|\alpha\beta\rangle_a \langle n_2|c_i c_j|0\rangle\end{aligned} \tag{7.79}$$

This TDA equation is also the shell model equation for two-hole states. It is usually written as,

$$\begin{aligned}&\omega(n_2)\langle n_2|c_\alpha c_\beta|0\rangle \\ =&(\varepsilon_\alpha+\varepsilon_\beta)\langle n_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle-\sum_{i<j}\langle ij|V|\alpha\beta\rangle_a\langle n_2|c_ic_j|0\rangle\end{aligned} \tag{7.80}$$

and the eigenvalues $\omega(n_2) = -(E_{n_2} - E_0)$ are minus the energies of the (A-2)-nucleus referred to the ground state of the A-nucleus, i. e. to the core. Remember that for convention these energies are minus the binding energies (with this convention the binding energies are all positive). The binding energy of a nucleus increases with the nuclear number A. Therefore $E_{n_2} - E_0 > 0$ and $\omega(n_2) < 0$. The eigenvalues of the TDA equation for the (A+2) nucleons, Eq. (7.77), are also negative, as it should be for bound states. The difference between particles and holes is that for holes the interaction contributes with a minus sign, as seen in Eq. (7.80).

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,

$$|n_2\rangle=\sum_{\alpha<\beta}X(\alpha\beta;n_2)c_\alpha^\dagger c_\beta^\dagger|0\rangle \tag{7.81}$$

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

$$\langle m_2|n_2\rangle=\delta_{m_2n_2}=\sum_{\alpha<\beta}X(\alpha\beta;n_2)\langle m_2|c_\alpha^\dagger c_\beta^\dagger|0\rangle \tag{7.82}$$

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

For a system with two particles in one orbital α, we simply have $\omega_{n_2} = 2\varepsilon_\alpha + \langle\alpha\alpha|V|\alpha\alpha\rangle^{JT}$ where JT denote the spin and isospin of the two particle state.

7.8 Homework problems

Exercise 1:

a) Write the operator $c_p^+ c_q$ in normal form.

b) Write the operator $c_p^+ c_q^+ c_r c_s$ in normal form.

Exercise 2:

a) Write the Hamiltonian $H = \sum_{\alpha\beta} < \alpha|T|\beta > c_\alpha^+ c_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} < \alpha\beta|V|\gamma\delta > c_\alpha^+ c_\beta^+ c_\delta c_\gamma$ in normal form and extract the Hartree-Fock potential.

b) Evaluate $< 0|H|0 >$.

Exercise 3:

Write the operator $: c_p^+ c_q^+ c_r c_s :: c_i^+ c_j^+ :$ in normal form.

Exercise 4:

a) With the Hamiltonian H written in the Hartree-Fock representation, i. e. $H = \sum_\alpha \epsilon_\alpha : c_\alpha^+ c_\alpha : + (1/2) \sum_{\alpha\beta\gamma\delta} < \alpha\beta|V|\gamma\delta >: c_\alpha^+ c_\beta^+ c_\delta c_\gamma :$ evaluate the commutator $[H, c_\alpha^+ c_\beta^+]$ in normal form and extract the two-particle RPA equation.

b) Starting from the RPA metric deduce the metric of the TDA space.