Chapter 3

Hartree-Fock Random-Phase Approximation

In this chapter we first present the Hartree-Fock method. This will be the starting point from which we drive the first- and second-order RPA formalism.

3.1 Hartree-Fock Method

The Hartree-Fock (HF) method is a so-called mean-field approximation. This means that the Hamiltonian of the nuclear many-body problem with A interacting particles (here the nucleons inside the nucleus) is reduced to an effective 1B operator. It is assumed that each particle moves independently of the other particles and is only affected by the global mean-field potential, determining its eigenenergy and eigenstate. Since the HF method does not account for any residual interaction between the particles there are no correlations between the different particles. Consequently, the many-body state of a HF calculation, $|\mathrm{HF}\rangle$, can be described by a single Slater-determinant (SD). The HF method is, therefore, one of the simplest approximations to the actual ground states of nuclei, and due to its simplicity also a computationally very cheap method. In this section, we will give an overview of the basic HF equations and properties, since these will in parts be used in the RPA formalism (see section 3.2).

In order to calculate the HF energies and states, we first need to take a look at the Hamiltonian under consideration. For a Hamiltonian $\hat{H}$ with a full 3B interaction we can write

$$\hat{H} = \hat{T} + \hat{V} + \hat{V}_{3\mathrm{N}} \tag{3.1}$$

$$= \sum_{i,i'} t_{i,i'}\, \hat{c}_i^\dagger \hat{c}_{i'} + \frac{1}{4} \sum_{ij,i'j'} v_{ij,i'j'}\, \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_{j'} \hat{c}_{i'} + \frac{1}{36} \sum_{ijk,i'j'k'} v^{3\mathrm{N}}_{ijk,i'j'k'}\, \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k^\dagger \hat{c}_{k'} \hat{c}_{j'} \hat{c}_{i'}, \tag{3.2}$$

Here the quantities $t_{i,i'}$, $v_{ij,i'j'}$ and $v^{3\mathrm{N}}_{ijk,i'j'k'}$ are antisymmetrized matrix elements of the kinetic energy, the 2B as well as the 3B interaction. The summation indices $i, j, k, i', \ldots$ run over the entire single-particle basis. At this point, the single-particle basis can be chosen arbitrarily. For practical applications, this is usually, as in this case, the harmonic oscillator (HO) basis. The HO basis states have several convenient properties which make them a suitable starting point. Taking the expectation value of the Hamiltonian $\hat{H}$ in the HF Slater-determinant $|\mathrm{HF}\rangle$ yields

the corresponding energy E

$$E = \langle \mathrm{HF}| \hat{H} |\mathrm{HF}\rangle = \langle \mathrm{HF}| \hat{T} + \hat{V} + \hat{V}^{3\mathrm{N}} |\mathrm{HF}\rangle \tag{3.3}$$

$$= \sum_{i,i'} t_{i,i'} \langle \mathrm{HF}| \hat{c}_i^\dagger \hat{c}_{i'} |\mathrm{HF}\rangle + \frac{1}{4} \sum_{ij,i'j'} v_{ij,i'j'} \langle \mathrm{HF}| \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_{j'} \hat{c}_{i'} |\mathrm{HF}\rangle + \frac{1}{36} \sum_{ijk,i'j'k'} v^{3\mathrm{N}}_{ijk,i'j'k'} \langle \mathrm{HF}| \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k^\dagger \hat{c}_{k'} \hat{c}_{j'} \hat{c}_{i'} |\mathrm{HF}\rangle , \tag{3.4}$$

where (3.2) has been inserted. We can now rewrite the expressions for the HF expectation values in (3.4) by introducing the 1B, 2B and 3B density matrices (for more information on density matrices see section 4.1)

$$\varrho_{i',i} = \langle \mathrm{HF}| \hat{c}_i^\dagger \hat{c}_{i'} |\mathrm{HF}\rangle , \tag{3.5}$$

$$\varrho_{i'j',ij} = \langle \mathrm{HF}| \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_{j'} \hat{c}_{i'} |\mathrm{HF}\rangle , \tag{3.6}$$

$$\varrho_{i'j'k',ijk} = \langle \mathrm{HF}| \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k^\dagger \hat{c}_{k'} \hat{c}_{j'} \hat{c}_{i'} |\mathrm{HF}\rangle , \tag{3.7}$$

which leads to a formula of the HF ground-state energy as functional of the density matrices

$$E[\varrho^1, \varrho^2, \varrho^3] = \sum_{i,i'} t_{i,i'} \varrho_{i',i} + \frac{1}{4} \sum_{ij,i'j'} v_{ij,i'j'} \varrho_{i'j',ij} + \frac{1}{36} \sum_{ijk,i'j'k'} v^{3\mathrm{N}}_{ijk,i'j'k'} \varrho_{i'j'k',ijk}. \tag{3.8}$$

Since the HF ground state $|\mathrm{HF}\rangle$ has the simple form of a single Slater-determinant, we can write the density matrices of higher particle-rank as a product of 1B density matrices (compare equation (4.34)). In combination with the sum and the coefficients from formula (3.4), the expression for the whole 2B term can be simplified as follows

$$\sum_{ij,i'j'} v_{ij,i'j'} \varrho_{i'j',ij} = \sum_{ij,i'j'} v_{ij,i'j'} \left(\varrho_{j',j} \varrho_{i',i} - \varrho_{j',i} \varrho_{i',j} \right) \tag{3.9}$$

$$= \sum_{ij,i'j'} \left(v_{ij,i'j'} \varrho_{j',j} \varrho_{i',i} - v_{ij,i'j'} \varrho_{j',i} \varrho_{i',j} \right) \tag{3.10}$$

$$= \sum_{ij,i'j'} \left(v_{ij,i'j'} \varrho_{j',j} \varrho_{i',i} - v_{ji,i'j'} \varrho_{j',j} \varrho_{i',i} \right) \tag{3.11}$$

$$= \sum_{ij,i'j'} \left(v_{ij,i'j'} \varrho_{j',j} \varrho_{i',i} + v_{ij,i'j'} \varrho_{j',j} \varrho_{i',i} \right) \tag{3.12}$$

$$= 2 \sum_{ij,i'j'} v_{ij,i'j'} \varrho_{j',j} \varrho_{i',i}, \tag{3.13}$$

where the indices i and j have been exchanged in (3.11) and the antisymmetry of $v_{ij,i'j'}$ has been used in (3.12). Analogously, we can simplify the 3B term, the corresponding density matrix then reads

$$\begin{aligned} \varrho_{i'j'k',ijk} = \quad & \varrho_{k',k} \left(\varrho_{i',i} \varrho_{j',j} - \varrho_{i',j} \varrho_{j',i} \right) \\ & + \varrho_{j',k} \left(\varrho_{i',j} \varrho_{k',i} - \varrho_{i',i} \varrho_{k',j} \right) \\ & + \varrho_{i',k} \left(\varrho_{k',j} \varrho_{j',i} - \varrho_{k',i} \varrho_{j',j} \right) . \end{aligned} \tag{3.14}$$

Inserting (3.14) into the 3B part of (3.8) leads to the following expression

$$\sum_{ijk,i'j'k'} v^{3\mathrm{N}}_{ijk,i'j'k'} \varrho_{i'j'k',ijk} = 6 \sum_{ijk,i'j'k'} v^{3\mathrm{N}}_{ijk,i'j'k'} \varrho_{k',k} \varrho_{i',i} \varrho_{j',j}. \tag{3.15}$$

With the above results, the HF ground-state energy E can now be written as a functional of only the 1B density matrix ϱ, as opposed to formula (3.8). For the energy we obtain

$$E[\varrho] = \sum_{i,i'} t_{i,i'}\, \varrho_{i',i} + \frac{1}{2} \sum_{ij,i'j'} v_{ij,i'j'}\, \varrho_{j',j}\, \varrho_{i',i} + \frac{1}{6} \sum_{ijk,i'j'k'} v^{\mathrm{3N}}_{ijk,i'j'k'}\, \varrho_{k',k}\, \varrho_{j',j}\, \varrho_{i',i}. \tag{3.16}$$

We will use the variational principle to determine the stationary point of $E[\varrho]$ with respect to ϱ. Varying the energy as in (3.16) with ϱ as the degree of freedom yields

$$\delta E[\varrho] = E[\varrho + \delta\varrho] - E[\varrho] \tag{3.17}$$

$$= \sum_{i,i'} t_{i,i'}\, \delta\varrho_{i',i} + \sum_{ij,i'j'} v_{ij,i'j'}\, \delta\varrho_{j',j}\, \varrho_{i',i} + \frac{1}{2} \sum_{\substack{ijk \\ i'j'k'}} v^{\mathrm{3N}}_{ijk,i'j'k'}\, \delta\varrho_{k',k}\, \varrho_{j',j}\, \varrho_{i',i}, \tag{3.18}$$

where terms involving higher orders in $\delta\varrho$ have been neglected. We can now factor out the part of expression (3.18) that carries the variation of the density matrix $\delta\varrho$, which yields

$$\delta E[\varrho] = \sum_{i,i'} \left(t_{i,i'} + \sum_{j,j'} v_{ij,i'j'}\, \varrho_{j',j} + \frac{1}{2} \sum_{jk,j'k'} v^{\mathrm{3N}}_{ijk,i'j'k'}\, \varrho_{j',j}\, \varrho_{k',k} \right) \delta\varrho_{i',i} \tag{3.19}$$

$$\equiv \sum_{i,i'} h_{i,i'}[\varrho]\, \delta\varrho_{i',i}. \tag{3.20}$$

The expression in parentheses in (3.19) defines the HF single-particle or mean-field Hamiltonian $\hat{h}[\varrho]$

$$h_{i,i'}[\varrho] \equiv t_{i,i'} + \sum_{j,j'} v_{ij,i'j'}\, \varrho_{j',j} + \frac{1}{2} \sum_{jk,j'k'} v^{\mathrm{3N}}_{ijk,i'j'k'}\, \varrho_{j',j}\, \varrho_{k',k}\,, \tag{3.21}$$

which is a 1B operator. It can be shown (cf. e.g. [RS80]) that the solution of the stationarity condition

$$\delta E[\varrho] = 0 \tag{3.22}$$

is equivalent to the solution of the eigenvalue problem of the mean-field Hamiltonian $\hat{h}[\varrho]$. That means we have to solve the equation

$$\hat{h}[\varrho]\, |i\rangle = \epsilon_i\, |i\rangle\,, \tag{3.23}$$

where, from now on, the $|i\rangle$ denote the single-particle HF basis states and ϵ_i the corresponding single-particle energies. In the following, the associated creation and annihilation operators in HF basis will be labeled $\hat{a}_i^\dagger$ and $\hat{a}_i$, respectively. Again, it has to be stressed that from this point on all the indices refer HF states and not HO states. In the HF basis, the 1B density matrix ϱ is equivalent to the identity matrix for all occupied states and zero otherwise. With that, the mean-field Hamiltonian simplifies even further to

$$h_{i,i'}[\varrho] = t_{i,i'} + \sum_{j}^{\mathrm{occ.}} v_{ij,i'j} + \frac{1}{2} \sum_{jk}^{\mathrm{occ.}} v^{\mathrm{3N}}_{ijk,i'jk}. \tag{3.24}$$

Note that the sums only run over the occupied states (denoted by "occ." above the sum symbol), which is caused by annihilators of unoccupied states acting on the HF vacuum: $\hat{a}_i\, |\mathrm{HF}\rangle = 0$, if $\epsilon_i > \epsilon_\mathrm{F}$, with the *Fermi energy* ϵ_F denoting the energy of the highest, still occupied state. By using (3.23) we obtain a connection between the matrix elements $h_{i,i'}[\varrho]$ of the mean-field Hamiltonian and its eigenenergies ϵ_i

$$h_{i,i'}[\varrho] = \langle i|\, \hat{h}[\varrho]\, |i'\rangle = \langle i|\, \epsilon_{i'}\, |i'\rangle = \epsilon_{i'}\, \langle i|i'\rangle = \epsilon_{i'}\, \delta_{ii'}, \tag{3.25}$$

and consequently an explicit formula for the single-particle energies

$$\epsilon_i = t_{i,i} + \sum_{j}^{\text{occ.}} v_{ij,ij} + \frac{1}{2} \sum_{jk}^{\text{occ.}} v^{\text{3N}}_{ijk,ijk}. \tag{3.26}$$

The ground-state energy in HF basis reads as follows (cf. (3.16), mind the difference of HO and HF basis)

$$E = \sum_{i}^{\text{occ.}} t_{i,i} + \frac{1}{2} \sum_{ij}^{\text{occ.}} v_{ij,ij} + \frac{1}{6} \sum_{ijk}^{\text{occ.}} v^{\text{3N}}_{ijk,ijk}, \tag{3.27}$$

and by using the formula for the single-particle energies (3.26), this can be rewritten into

$$E = \sum_{i}^{\text{occ.}} \epsilon_i - \frac{1}{2} \sum_{ij}^{\text{occ.}} v_{ij,ij} - \frac{1}{3} \sum_{ijk}^{\text{occ.}} v^{\text{3N}}_{ijk,ijk}. \tag{3.28}$$

With (3.28) we now finally have a formula for the total energy of the A-nucleon system, described via a Hamiltonian that contains a full 3B interaction, in HF approximation.

3.2 Random-Phase Approximation

The random-phase approximation (RPA) is a standard tool for the investigation of excited collective states. Its framework is built on the results of a preceding HF calculation, i.e., it uses the single-particle states of such a calculation (HF-RPA). Within the RPA, all excited states are computed via linear combinations of particle-hole (ph) excitations of the RPA ground state. In particular, the RPA ground state already contains correlations and has, therefore, a far more complicated structure than the simple HF Slater-determinant.

3.2.1 Particle-Hole Formalism

It has already been stated that within RPA, the ground state as well as excited states are obtained via ph excitations of the HF state, therefore, the RPA is referred to as a *particle-hole theory*. Since the concept of ph excitations will be essential to all of the following calculations involving the RPA framework, this section is dedicated to a short introduction to the ph formalism that will be needed later on. In the following, all indices $i, j, p, h, ...$ shall denote HF single-particle states.

In second quantization, a ph excitation is described as follows: One particle in a state $|h\rangle$ below the Fermi energy ϵ_{F} is destroyed by application of an annihilation operator $\hat{a}_h$, while at the same time an unoccupied state $|p\rangle$ above the Fermi energy will be populated with a particle by applying a creation operator $\hat{a}_p^\dagger$. Together, this creator-annihilator pair corresponds to an excitation of a particle from the initial state $|h\rangle$ to the final state $|p\rangle$. One such pair defines a 1-particle-1-hole (1p1h) excitation. If two, three or n creator-annihilator pairs act on a state, we analogously call these 2p2h, 3p3h or npnh excitations, respectively. A schematic view of a 1p1h excitation is depicted in Figure 3.1.

Due to the fact that we excite a particle from a state below ϵ_{F} to a state above ϵ_{F}, physically speaking, these ph excitations cost a certain amount of energy, which is given by the difference of the single-particle energies. In the case described above, this would correspond to

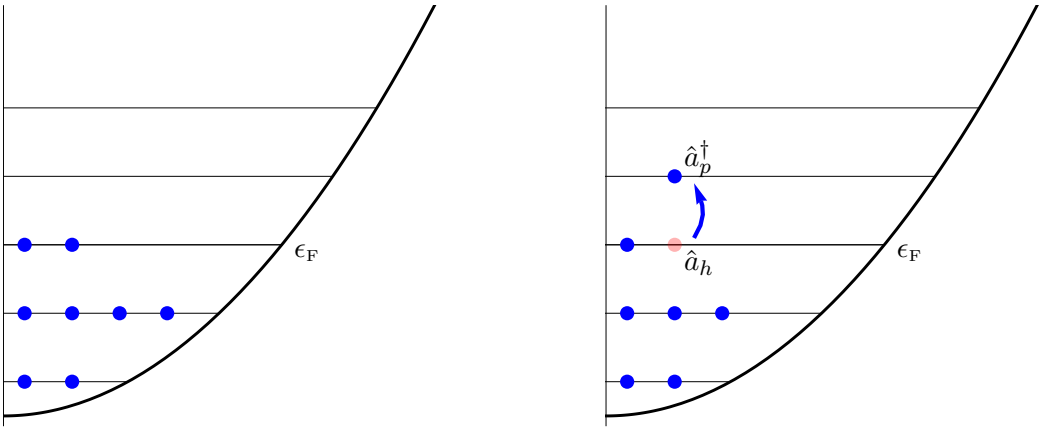
$$\epsilon_{ph} \equiv \epsilon_p - \epsilon_h, \tag{3.29}$$

with ϵ_i being the HF single-particle energy of the state $|i\rangle$ (see (3.26)).

So far we have concerned ourselves only with performing ph excitations. In principle the reversed process, which would be a hole-particle (hp) excitation is of course possible as well. Here, we would annihilate a particle in a state above ϵ_{F} and create one in a state below it. Energetically speaking, this corresponds to a de-excitation which frees energy, in magnitude equal to (3.29). Obviously, such a process can only take place if a matching pair of states is (un-)occupied. More specifically, this is *not* the case for any single Slater-determinant, including $|\text{HF}\rangle$. Mind that in contrast to the hp process, the initially discussed ph excitation is always possible on SDs.

The above discussion suggests a rigid partitioning of the HF basis into two categories, since the states above and below the Fermi energy play different roles in (de-)excitations. This consideration leads to the following convention for the HF indices, which shall be used throughout this thesis unless explicitly stated otherwise:

- Single-particle states **below** the Fermi energy, i.e., "hole" states: $h, h', ...$
- Single-particle states **above** the Fermi energy, i.e., "particle" states: $p, p', ...$
- **All** single-particle states: $i, j, ...$



(a) Ground state. (b) Particle-hole excitation.

Figure 3.1: Particle-hole excitation. Figure (a) shows the nucleus in the HF ground state with the Fermi energy ϵ_{F}. In figure (b) we have a similar situation only now with a ph excitation $\hat{a}_p^\dagger \hat{a}_h$ that annihilates a particle in the state $|h\rangle$ below the Fermi energy and creates one in the state $|p\rangle$ above the Fermi energy.

Hence, all (de-)excitations are realized by the application of pairs of fermion operators, either of the sort $\hat{a}_p^\dagger \hat{a}_h$ for excitations or $\hat{a}_h^\dagger \hat{a}_p$ for de-excitations, respectively. Note that this partitioning of our basis is only applicable to nuclei with so-called *subshell closures* where all j orbitals are either completely occupied or entirely unoccupied. If an orbital is partially filled, both excitation and de-excitation operations can be performed and no clear distinction between particle and hole states is possible. In the next section, we will use this ph formalism to derive the basic RPA equations.

3.2.2 Derivation of the basic RPA Equations

In this section the RPA equations shall be derived using the so-called *equations of motion* (EOM) method. The notation and the steps of the derivation are taken from [Suh07]. Within the EOM method the actual calculation of the RPA ground state, which we denote $|\mathrm{RPA}\rangle$, is avoided. For now, this state will only be written implicitly. In order to obtain generic expressions for the ground state $|\mathrm{RPA}\rangle$, we can define *excitation creation operators* (ECO) $\hat{Q}_\omega^\dagger$. These $\hat{Q}_\omega^\dagger$ are intended to create an *excited state* $|\omega\rangle$ when applied to the RPA ground state, i.e.

$$|\omega\rangle \equiv \hat{Q}_\omega^\dagger |\mathrm{RPA}\rangle \,, \tag{3.30}$$

where ω is a short-hand notation for a set of quantum numbers, usually $\omega = (n, J^\pi, M)$, with n being the number of the excited state, J the angular momentum, M the z-projection and π the parity. We usually investigate different angular momenta and parities separately, so when later we write sums over ω this simply implies a sum over n. The corresponding annihilator $\hat{Q}_\omega$ obviously de-excites the associated excited state back to the ground state

$$\hat{Q}_\omega |\omega\rangle = |\mathrm{RPA}\rangle \,. \tag{3.31}$$

When applied to the energetically lowest state, the ground state, further de-excitation is unphysical, thus,

$$\hat{Q}_\omega |\mathrm{RPA}\rangle \equiv 0, \quad \forall\, \omega. \tag{3.32}$$

Expressions (3.30) and (3.32) are the defining relations for the ECOs $\hat{Q}^\dagger_\omega$ as well as for the ground state $|\mathrm{RPA}\rangle$. We stress that the whole set of ECOs $\hat{Q}^\dagger_\omega$ together with the ground state $|\mathrm{RPA}\rangle$ and the excitation energies E^{RPA}_ω define the complete solution to the RPA problem. From these defining relations also the orthogonality of the excited state to the ground state follows:

$$\langle \mathrm{RPA}|\omega\rangle = \langle \mathrm{RPA}|\, \hat{Q}^\dagger_\omega\, |\mathrm{RPA}\rangle = \langle \mathrm{RPA}|\, \hat{Q}_\omega\, |\mathrm{RPA}\rangle^* \equiv 0, \quad \forall\, \omega. \tag{3.33}$$

Formally, the ECOs can be written as $\hat{Q}^\dagger_\omega = |\omega\rangle\langle \mathrm{RPA}|$. However, this is just a generic notation which in itself does not provide any practical assistance for the actual solution of the RPA problem. In fact, the detailed form of the ECOs depends on the type of RPA that is used. Up to this point we have made no restrictions for these operators. In section 3.2.3 we will discuss the most simple form of RPA and its corresponding ECOs.

For the EOM derivation of the RPA equations, it is helpful to first take a look at the stationary Schrödinger equation

$$\hat{H}\, |\mathrm{RPA}\rangle = E_0\, |\mathrm{RPA}\rangle\,, \tag{3.34}$$

$$\hat{H}\, |\omega\rangle = E_\omega\, |\omega\rangle \quad \forall\omega, \tag{3.35}$$

where the RPA ground-state energy has been labeled E_0 and the energies of the excited states E_ω. With the use of (3.30), (3.35) can be rewritten as

$$\hat{H}\hat{Q}^\dagger_\omega\, |\mathrm{RPA}\rangle = E_\omega \hat{Q}^\dagger_\omega\, |\mathrm{RPA}\rangle. \tag{3.36}$$

We can also evaluate the interchanged term on the left-hand side of (3.36), i.e.

$$\hat{Q}^\dagger_\omega \hat{H}\, |\mathrm{RPA}\rangle = \hat{Q}^\dagger_\omega E_0\, |\mathrm{RPA}\rangle = E_0 \hat{Q}^\dagger_\omega\, |\mathrm{RPA}\rangle\,. \tag{3.37}$$

Subtracting (3.37) from (3.36) then yields

$$\hat{H}\hat{Q}^\dagger_\omega\, |\mathrm{RPA}\rangle - \hat{Q}^\dagger_\omega \hat{H}\, |\mathrm{RPA}\rangle = E_\omega \hat{Q}^\dagger_\omega\, |\mathrm{RPA}\rangle - E_0 \hat{Q}^\dagger_\omega\, |\mathrm{RPA}\rangle \tag{3.38}$$

$$\left(\hat{H}\hat{Q}^\dagger_\omega - \hat{Q}^\dagger_\omega \hat{H}\right) |\mathrm{RPA}\rangle = (E_\omega - E_0)\hat{Q}^\dagger_\omega\, |\mathrm{RPA}\rangle \tag{3.39}$$

$$[\hat{H}, \hat{Q}^\dagger_\omega]\, |\mathrm{RPA}\rangle = (E_\omega - E_0)\hat{Q}^\dagger_\omega\, |\mathrm{RPA}\rangle\,, \tag{3.40}$$

where we have introduced the commutator between $\hat{H}$ and $\hat{Q}^\dagger_\omega$. At this point it is convenient to introduce a new quantity, the RPA excitation energy E^{RPA}_ω given by

$$E^{\mathrm{RPA}}_\omega \equiv E_\omega - E_0, \tag{3.41}$$

i.e., the energy of the state $|\omega\rangle$ relative to the ground state $|\mathrm{RPA}\rangle$. With this, (3.40) becomes

$$[\hat{H}, \hat{Q}^\dagger_\omega]\, |\mathrm{RPA}\rangle = E^{\mathrm{RPA}}_\omega \hat{Q}^\dagger_\omega\, |\mathrm{RPA}\rangle\,. \tag{3.42}$$

Relation (3.42) is the so-called *equation of motion* for the excitation creation operators $\hat{Q}^\dagger_\omega$. As mentioned before, in order to actually determine a solution for the operators $\hat{Q}^\dagger_\omega$, we first need to make an ansatz for their structure. The different types of ECOs will be the topic of the next section. Afterwards, we will proceed by solving (3.42) with the help of the variational method.

3.2.3 First-Order ECOs

As already stated in section 3.2.2, the detailed form for the ECOs depends on the type of RPA that is used for the calculations. As a start, we will deal with the *standard* or *first-order* RPA. The first-order RPA is defined by the fact that its ECOs perform only 1p1h (de-)excitations on the ground state $|\mathrm{RPA}\rangle$. So, in summary, the first-order ECOs should

- allow for 1p1h excitations ($\hat{a}_p^\dagger \hat{a}_h$),
- allow for 1p1h de-excitations ($\hat{a}_h^\dagger \hat{a}_p$),
- provide the correct quantum numbers.

Higher-order excitations (2p2h, ...) will of course yield a better description of the system since they allow for more degrees of freedom, but at the same time they are connected to a more complicated formalism. For now we will stick to 1p1h excitations, the natural extension to 2p2h contributions will be discussed in section 3.3.

Earlier we defined ω to be $\omega = (n, J^\pi, M)$. It is convenient to ensure that the pair of fermion operators for (de-)excitations is coupled to the correct angular momentum J with z-component M. This is why, usually, the ECOs do not contain uncoupled pairs of fermion operators but rather the coupled versions. When coupling two single angular momenta to a total angular momentum, this corresponds to a replacement of the two quantum numbers for the single z-components, m_1 and m_2, with the total angular momentum J and its (total) z-component M. In order to express this in the formulae, we introduce a new notation, dividing the quantum numbers which characterize a single-particle state i into one part containing only its z-component, m_i, and one part containing all the remaining "m-less" quantum numbers $\bar{i}$:

$$i \equiv (\bar{i}, m_i). \tag{3.43}$$

We define the coupled product of a pair of fermion operators $\hat{a}_{\bar{p}}^\dagger$ and $\hat{\tilde{a}}_{\bar{h}}$ (see below) as

$$\hat{\mathcal{A}}_{\bar{p}\bar{h}}^\dagger(JM) \equiv [\hat{a}_{\bar{p}}^\dagger \hat{\tilde{a}}_{\bar{h}}]_{JM}, \tag{3.44}$$

where the *tensor product* of two spherical tensors $\boldsymbol{T}_{j_1}$ and $\boldsymbol{T}_{j_2}$ of rank j_1 and j_2 and with components T_{j_1,m_1} and T_{j_2,m_2}, respectively, is given by

$$T_{JM} = [\boldsymbol{T}_{j_1} \boldsymbol{T}_{j_2}]_{JM} = \sum_{m_1,m_2} C(j_1 m_1, j_2 m_2 | JM) T_{j_1 m_1} T_{j_2 m_2}, \tag{3.45}$$

yielding the $2M+1$ components T_{JM} of a new spherical tensor $\boldsymbol{T}_J$ of rank J, with the quantity $C(j_1 m_1, j_2 m_2 | JM)$ denoting a Clebsch-Gordan coefficient. The use of the "tilde" operator $\hat{\tilde{a}}_i$ in (3.44) defined via

$$\hat{\tilde{a}}_i \equiv (-1)^{j_i + m_i}\, \hat{a}_{\bar{i},-m_i}, \tag{3.46}$$

is necessary, because the regular annihilation operator $\hat{a}_i$ is not a spherical tensor operator, and hence it cannot be used for the tensor product. Including the factor $(-1)^{j_i+m_i}$ and changing the sign of the z-component of the operator yields the spherical tensor operator $\hat{\tilde{a}}_i$, as required by (3.45). A more detailed discussion of spherical tensor operators can be found in Appendix A. Following this, the expression $[\hat{a}_{\bar{p}}^\dagger \hat{\tilde{a}}_{\bar{h}}]_{JM}$ is the tensor product of two spherical tensors $\hat{a}_{\bar{p}}^\dagger$ and $\hat{\tilde{a}}_{\bar{h}}$ of rank j_p and j_h, respectively. With the help of (3.45) we can write the new coupled excitation

operator (3.44) as

$$\hat{\mathcal{A}}^\dagger_{\bar{p}\bar{h}}(JM) = [\hat{a}^\dagger_{\bar{p}}\hat{\tilde{a}}_{\bar{h}}]_{JM} \tag{3.47}$$

$$= \sum_{m_p,m_h} (-1)^{j_h+m_h}\, C(j_p m_p, j_h m_h|JM)\, \hat{a}^\dagger_{\bar{p},m_p}\hat{a}_{\bar{h},\text{-}m_h} \tag{3.48}$$

$$= \sum_{m_p,m_h} (-1)^{j_h-m_h}\, C(j_p m_p, j_h \text{-}m_h|JM)\, \hat{a}^\dagger_{\bar{p},m_p}\hat{a}_{\bar{h},m_h} \tag{3.49}$$

$$= \sum_{m_p,m_h} (-1)^{j_h-m_h}\, C(j_p m_p, j_h \text{-}m_h|JM)\, \hat{\mathcal{A}}^\dagger_{ph}, \tag{3.50}$$

where we introduced the uncoupled ph creation operator $\hat{\mathcal{A}}^\dagger_{ph} = \hat{a}^\dagger_p\hat{a}_h$. Note that the Hermitian conjugate of the coupled ph operator, $\hat{\mathcal{A}}_{\bar{p}\bar{h}}(JM)$, is not a spherical tensor operator, but analogously to the case of the simple particle creators and annihilators we can construct a coupled annihilator, which then is a spherical tensor operator, as follows

$$\hat{\tilde{\mathcal{A}}}_{\bar{p}\bar{h}}(JM) \equiv (-1)^{J+M}\hat{\mathcal{A}}_{\bar{p}\bar{h}}(J\text{-}M), \tag{3.51}$$

which shows the exact same modifications as (3.46). Owing to spherical symmetry, in practical applications it suffices to calculate only one of the $\hat{\mathcal{A}}_{\bar{p}\bar{h}}(JM)$. Choosing $M = 0$ yields the convenient property that the spherical, "tilde" annihilators relate directly to their non-spherical counterparts:

$$\hat{\tilde{\mathcal{A}}}_{\bar{p}\bar{h}}(J0) = (-1)^J\hat{\mathcal{A}}_{\bar{p}\bar{h}}(J0). \tag{3.52}$$

With (3.44) and (3.51), we can write the most general form for the *coupled* first-order ECO as

$$\hat{Q}^\dagger_\omega = \sum_{\bar{p},\bar{h}} \left(X^\omega_{\bar{p}\bar{h}}\, \hat{\mathcal{A}}^\dagger_{\bar{p}\bar{h}}(JM) - Y^\omega_{\bar{p}\bar{h}}\, \hat{\tilde{\mathcal{A}}}_{\bar{p}\bar{h}}(JM) \right), \tag{3.53}$$

where the sums run over all occupied states (h) and all unoccupied states (p), respectively. The term $\hat{\mathcal{A}}^\dagger_{\bar{p}\bar{h}}(JM)$ describes a single ph excitation process, while the term $\hat{\tilde{\mathcal{A}}}_{\bar{p}\bar{h}}(JM)$ accomplishes the inverse process, which means a *hp excitation* or *de-excitation* (cf. section 3.2.1). Both these processes can occur and contribute to a certain degree to the excited state $|\omega\rangle$ which is given by the corresponding coefficients ($X^\omega_{\bar{p}\bar{h}}$, $Y^\omega_{\bar{p}\bar{h}}$). These coefficients are usually referred to as *RPA amplitudes*. The uncoupled analogon of (3.53) reads

$$\hat{Q}^\dagger_\omega = \sum_{p,h} \left(X^\omega_{ph}\, \hat{\mathcal{A}}^\dagger_{ph} - Y^\omega_{ph}\, \hat{\mathcal{A}}_{ph} \right). \tag{3.54}$$

Note that the amplitudes in (3.53) and (3.54) are, strictly speaking, not identical, since the first ones refer to the contributions from coupled ph excitations, the latter ones to contributions from the uncoupled excitations. We choose not to introduce a separate notation for the forward (X^ω) and backward (Y^ω) amplitudes of coupled and uncoupled ECOs, since their physical meaning remains the same. The question of coupling is addressed via their index notations, i.e., compare $X^\omega_{\bar{p}\bar{h}}$ to X^ω_{ph}. The uncoupled variant greatly helps in keeping equations lucid. The following discussion is therefore given in an uncoupled formulation. The conversion to coupled expressions will be done only for our final results (see section 3.2.9).

At this point, a remark on the form of the ECO as in (3.54) seems suitable. As stated earlier, the second term allows for hp excitations (or de-excitations). This degree of freedom is directly responsible for the fact that, in general, the RPA ground state $|\text{RPA}\rangle$ is not the simple HF

ground state $|\mathrm{HF}\rangle$. To see this, we could assume that the RPA ground state was indeed $|\mathrm{HF}\rangle$. The application of the annihilator $\hat{Q}_\omega$ on $|\mathrm{HF}\rangle$ would then yield

$$\hat{Q}_\omega |\mathrm{HF}\rangle = \sum_{p,h} \left(X_{ph}^{\omega\,*}\, \hat{a}_h^\dagger \hat{a}_p - Y_{ph}^{\omega\,*}\, \hat{a}_p^\dagger \hat{a}_h \right) |\mathrm{HF}\rangle \tag{3.55}$$

$$= \sum_{p,h} \Big(X_{ph}^{\omega\,*}\, \underbrace{\hat{a}_h^\dagger \hat{a}_p |\mathrm{HF}\rangle}_{=0} - Y_{ph}^{\omega\,*}\, \hat{a}_p^\dagger \hat{a}_h |\mathrm{HF}\rangle \Big) \tag{3.56}$$

$$= -\sum_{p,h} Y_{ph}^{\omega\,*}\, \hat{a}_p^\dagger \hat{a}_h |\mathrm{HF}\rangle\,, \tag{3.57}$$

which generally evaluates to a non-zero value (except for the trivial case that all Y_{ph}^ω are zero). This is in contradiction to the defining relation (3.32), and consequently we find $|\mathrm{HF}\rangle \neq |\mathrm{RPA}\rangle$ for all non-trivial cases. In fact, a model exists where there are no amplitudes Y_{ph}^ω within the ECOs. It is called the Tamm-Dancoff Approximation, which we will briefly discuss in section 3.2.6.

3.2.4 Variational Principle and Quasi-Boson Approximation

Since all excited states $|\omega\rangle$ are orthogonal to the ground state (cf. (3.33)), let us consider a variation $\delta\hat{Q}^\dagger$ of the ECOs $\hat{Q}_\omega^\dagger$. This variation is supposed to span the full model space, with the condition that it still has to be orthogonal to the ground state, i.e.

$$\delta\hat{Q} |\mathrm{RPA}\rangle = 0. \tag{3.58}$$

For first-order RPA this variation can be written as

$$\delta\hat{Q} = \sum_{p,h} \left(\delta X_{ph}^*\, \hat{a}_h^\dagger \hat{a}_p - \delta Y_{ph}^*\, \hat{a}_p^\dagger \hat{a}_h \right). \tag{3.59}$$

We can calculate the overlap of $\langle \delta Q|$ with the EOM expression (3.42), which yields

$$\langle \mathrm{RPA}| \,\delta\hat{Q}[\hat{H}, \hat{Q}_\omega^\dagger] |\mathrm{RPA}\rangle = E_\omega^{\mathrm{RPA}} \langle \mathrm{RPA}| \,\delta\hat{Q}\hat{Q}_\omega^\dagger |\mathrm{RPA}\rangle\,. \tag{3.60}$$

A commutator can be introduced by use of the orthogonality relation (3.58) between the variation and the ground state, leading to

$$\langle \mathrm{RPA}| \,[\delta\hat{Q}, [\hat{H}, \hat{Q}_\omega^\dagger]] |\mathrm{RPA}\rangle = E_\omega^{\mathrm{RPA}} \langle \mathrm{RPA}| \,[\delta\hat{Q}, \hat{Q}_\omega^\dagger] |\mathrm{RPA}\rangle\,, \tag{3.61}$$

which is the general form for the equation of motion. The advantage of (3.61) is that systematically improved extensions for the ECOs can be introduced. We will revisit the above equation later when dealing with second-order RPA. For now we proceed with the first-order ECOs and insert $\delta\hat{Q}$ and $\hat{Q}_\omega^\dagger$ into (3.61). This equation holds for arbitrary variations δQ. We bring to mind that the ph excitations are linearly independent from each other and of course also from the hp excitations. The variational ansatz of (3.61), therefore, leads to a number of separate identities, one for each ph excitation and one for each de-excitation. With this, we get two different sets of equations for each ω, p, h:

$$\delta X_{ph}: \quad \langle \mathrm{RPA}| \,[\hat{a}_h^\dagger \hat{a}_p, [\hat{H}, \hat{Q}_\omega^\dagger]] |\mathrm{RPA}\rangle = E_\omega^{\mathrm{RPA}} \langle \mathrm{RPA}| \,[\hat{a}_h^\dagger \hat{a}_p, \hat{Q}_\omega^\dagger] |\mathrm{RPA}\rangle\,, \tag{3.62}$$

$$\delta Y_{ph}: \quad \langle \mathrm{RPA}| \,[\hat{a}_p^\dagger \hat{a}_h, [\hat{H}, \hat{Q}_\omega^\dagger]] |\mathrm{RPA}\rangle = E_\omega^{\mathrm{RPA}} \langle \mathrm{RPA}| \,[\hat{a}_p^\dagger \hat{a}_h, \hat{Q}_\omega^\dagger] |\mathrm{RPA}\rangle\,. \tag{3.63}$$

The first set (3.62) results from the term carrying the δX amplitudes. Analogously, the second set (3.63) comes from the δY amplitudes.

At this point, we have reached the end of the exact, analytical derivation of the EOMs. The reason for this is the fact that all the ECOs $\hat{Q}^\dagger_\omega$ as well as the ground state $|\mathrm{RPA}\rangle$ depend on each other (cf. section 3.2.2). As a consequence, we are not able to answer, a priori, the question what the application of, e.g., $\hat{a}^\dagger_i$ on $|\mathrm{RPA}\rangle$ will yield. Therefore, the only possibility to solve the above equations would be via an *iterative scheme*: We would have to guess a solution, plug it into the corresponding equations, and from that obtain a new solution. This would have to be done until we achieve a solution which is self-consistent (to a chosen accuracy). Usually, one will not undergo the trouble of self-consistency to solve the RPA equations, this procedure is chosen only in the so-called *self-consistent RPA* [Cat+96].

In order to be able to simplify these equations further, we introduce the *quasi-boson approximation* (QBA). Since we always have pairs (even numbers) of fermion operators in the RPA equations, we can naively assume them to behave at least roughly as *Bose-like* operators. An odd number of fermion operators on the other hand could be considered to behave roughly as *Fermi-like* operators. We can evaluate the commutator of two Bose-like fermion pairs with the help of the basic commutator relations for fermions. This gives us

$$[\hat{a}^\dagger_p\hat{a}_h, \hat{a}^\dagger_{h'}\hat{a}_{p'}] = \delta_{hh'}\,\hat{a}^\dagger_p\hat{a}_{p'} - \delta_{pp'}\,\hat{a}^\dagger_{h'}\hat{a}_h, \tag{3.64}$$

which is an exact operator identity. Within the QBA, the simplification is made that expectation values of commutators of this sort are replaced by their HF expectation value, i.e.

$$\begin{aligned}
\langle\mathrm{RPA}|\,[\hat{a}^\dagger_p\hat{a}_h, \hat{a}^\dagger_{h'}\hat{a}_{p'}]\,|\mathrm{RPA}\rangle &\overset{\mathrm{QBA}}{\approx} \langle\mathrm{HF}|\,[\hat{a}^\dagger_p\hat{a}_h, \hat{a}^\dagger_{h'}\hat{a}_{p'}]\,|\mathrm{HF}\rangle &(3.65)\\
&= \langle\mathrm{HF}|\,\delta_{hh'}\,\hat{a}^\dagger_p\hat{a}_{p'} - \delta_{pp'}\,\hat{a}^\dagger_{h'}\hat{a}_h\,|\mathrm{HF}\rangle &(3.66)\\
&= -\delta_{pp'}\delta_{hh'}. &(3.67)
\end{aligned}$$

Interestingly, this looks just like the basic commutator relation between two bosonic operators $\hat{b}^\dagger_j$ and $\hat{b}_i$, given by

$$[\hat{b}_i, \hat{b}^\dagger_j] = \delta_{ij}, \tag{3.68}$$

which can be seen by defining new operators for the Bose-like terms, i.e.

$$\begin{aligned}
B_i &\equiv \hat{a}^\dagger_{h'}\hat{a}_{p'}, \quad i = (h', p'), &(3.69)\\
B^\dagger_j &= \hat{a}^\dagger_p\hat{a}_h, \quad j = (h, p), &(3.70)
\end{aligned}$$

with the matching orthogonality relation $\delta_{ij} = \delta_{hh'}\,\delta_{pp'}$. We see that replacing expectation values of the sort (3.64) by their HF expectation values leads to expressions which look like the result of the commutator between two bosonic operators, hence the name quasi-boson approximation. In summary, the QBA can be considered as the approximation

$$\langle\mathrm{RPA}|\,\hat{O}_{\text{Bose-like}}\,|\mathrm{RPA}\rangle \approx \langle\mathrm{HF}|\,\hat{O}_{\text{Bose-like}}\,|\mathrm{HF}\rangle\,.$$

The replacement of the expectation value $\langle\mathrm{RPA}|\ldots|\mathrm{RPA}\rangle$ with its $|\mathrm{HF}\rangle$ pendant is justified by the assumption that pairs of fermion operators behave similar to the way bosonic operators would do. However, by performing this replacement we are neglecting some of the operator terms, and, therefore, it remains to be seen whether or not this assumption is a reasonable one.

In order to get a better understanding of the QBA, we will consider the $|\mathrm{RPA}\rangle$ expectation value of the right-hand side of (3.62). Inserting definition (3.54) for the ECO yields

$$\langle \mathrm{RPA}| \left[\hat{a}_h^\dagger \hat{a}_p, \hat{Q}_\omega^\dagger\right] |\mathrm{RPA}\rangle = \sum_{p'h'} X_{p'h'}^\omega \langle \mathrm{RPA}| \left[\hat{a}_h^\dagger \hat{a}_p, \hat{a}_{p'}^\dagger \hat{a}_{h'}\right] |\mathrm{RPA}\rangle + 0 \tag{3.71}$$

$$= \sum_{p'h'} X_{p'h'}^\omega \Big(\delta_{p,p'}\delta_{h,h'} - \delta_{p,p'} \langle \mathrm{RPA}| \hat{a}_{h'} \hat{a}_h^\dagger |\mathrm{RPA}\rangle - \delta_{h,h'} \langle \mathrm{RPA}| \hat{a}_{p'}^\dagger \hat{a}_p |\mathrm{RPA}\rangle \Big) \tag{3.72}$$

$$= X_{ph}^\omega - \sum_{h'} X_{ph'}^\omega \langle \mathrm{RPA}| \hat{a}_{h'} \hat{a}_h^\dagger |\mathrm{RPA}\rangle - \sum_{p'} X_{p'h}^\omega \langle \mathrm{RPA}| \hat{a}_{p'}^\dagger \hat{a}_p |\mathrm{RPA}\rangle . \tag{3.73}$$

If there are no phase correlations between the expectation values and the amplitudes, the last two terms in (3.73) can be expected to be small. Hence the name *random*-phase approximation. Generally, we can assume the QBA to be a reasonable approximation if the RPA ground state $|\mathrm{RPA}\rangle$ does not differ too much from the HF ground state $|\mathrm{HF}\rangle$, i.e., if the ground-state correlations are relatively weak.

3.2.5 RPA Equations

Applying the QBA to (3.62) and (3.63) yields

$$\langle \mathrm{HF}| \left[\hat{a}_h^\dagger \hat{a}_p, [\hat{H}, \hat{Q}_\omega^\dagger]\right] |\mathrm{HF}\rangle = E_\omega^{\mathrm{RPA}} \langle \mathrm{HF}| \left[\hat{a}_h^\dagger \hat{a}_p, \hat{Q}_\omega^\dagger\right] |\mathrm{HF}\rangle , \tag{3.74}$$

$$\langle \mathrm{HF}| \left[\hat{a}_p^\dagger \hat{a}_h, [\hat{H}, \hat{Q}_\omega^\dagger]\right] |\mathrm{HF}\rangle = E_\omega^{\mathrm{RPA}} \langle \mathrm{HF}| \left[\hat{a}_p^\dagger \hat{a}_h, \hat{Q}_\omega^\dagger\right] |\mathrm{HF}\rangle . \tag{3.75}$$

The advantage of this is that we now know exactly what the application of each of the fermion operators to the HF state $|\mathrm{HF}\rangle$ will yield. Therefore, with the help of the QBA, a number simplifications are possible. Taking a look at the right-hand side of (3.74) shows that the second term of the commutator vanishes, since $\hat{a}_p |\mathrm{HF}\rangle = 0$. Similarly, the first term of the commutator on the right-hand side of (3.75) vanishes due to the fact that $\langle \mathrm{HF}| \hat{a}_p^\dagger = 0$. The same, of course, holds true for both of the outer commutators on the left-hand sides of (3.74) and (3.75), respectively. For the moment we are left with the following sets of equations

$$\langle \mathrm{HF}| \hat{a}_h^\dagger \hat{a}_p [\hat{H}, \hat{Q}_\omega^\dagger] |\mathrm{HF}\rangle = E_\omega^{\mathrm{RPA}} \langle \mathrm{HF}| \hat{a}_h^\dagger \hat{a}_p \hat{Q}_\omega^\dagger |\mathrm{HF}\rangle , \tag{3.76}$$

$$\langle \mathrm{HF}| [\hat{H}, \hat{Q}_\omega^\dagger] \hat{a}_p^\dagger \hat{a}_h |\mathrm{HF}\rangle = E_\omega^{\mathrm{RPA}} \langle \mathrm{HF}| \hat{Q}_\omega^\dagger \hat{a}_p^\dagger \hat{a}_h |\mathrm{HF}\rangle . \tag{3.77}$$

We can now insert our choice for the ECOs as in (3.54) into the above equations. Doing this for the matrix element on the right-hand side of (3.76) yields

$$\langle \mathrm{HF}| \hat{a}_h^\dagger \hat{a}_p \hat{Q}_\omega^\dagger |\mathrm{HF}\rangle = \sum_{p'h'} \left(X_{p'h'}^\omega \langle \mathrm{HF}| \hat{a}_h^\dagger \hat{a}_p \hat{a}_{p'}^\dagger \hat{a}_{h'} |\mathrm{HF}\rangle - Y_{p'h'}^\omega \langle \mathrm{HF}| \hat{a}_h^\dagger \hat{a}_p \hat{a}_{h'}^\dagger \hat{a}_{p'} |\mathrm{HF}\rangle \right) \tag{3.78}$$

$$= \sum_{p'h'} \left(X_{p'h'}^\omega \cdot \delta_{hh'}\delta_{pp'} - Y_{p'h'}^\omega \cdot 0 \right) \tag{3.79}$$

$$= X_{ph}^\omega , \tag{3.80}$$

Similarly, for the matrix element on the right-hand side of (3.77) we obtain

$$\langle \mathrm{HF}| \hat{Q}^\dagger_\omega \, \hat{a}^\dagger_p \hat{a}_h \, |\mathrm{HF}\rangle = \sum_{p'h'} \Big(X^\omega_{p'h'} \, \langle \mathrm{HF}| \, \hat{a}^\dagger_{p'} \hat{a}_{h'} \hat{a}^\dagger_p \hat{a}_h \, |\mathrm{HF}\rangle - Y^\omega_{p'h'} \, \langle \mathrm{HF}| \, \hat{a}^\dagger_{h'} \hat{a}_{p'} \hat{a}^\dagger_p \hat{a}_h \, |\mathrm{HF}\rangle \Big) \tag{3.81}$$

$$= \sum_{p'h'} \Big(X^\omega_{p'h'} \cdot 0 - Y^\omega_{p'h'} \cdot \delta_{hh'} \delta_{pp'} \Big) \tag{3.82}$$

$$= -Y^\omega_{ph}. \tag{3.83}$$

As an intermediate result, we end up with

$$\langle \mathrm{HF}| \, \hat{a}^\dagger_h \hat{a}_p [\hat{H}, \hat{Q}^\dagger_\omega] \, |\mathrm{HF}\rangle = \quad E^{\mathrm{RPA}}_\omega X^\omega_{ph}, \tag{3.84}$$

$$\langle \mathrm{HF}| \, [\hat{H}, \hat{Q}^\dagger_\omega] \hat{a}^\dagger_p \hat{a}_h \, |\mathrm{HF}\rangle = -E^{\mathrm{RPA}}_\omega Y^\omega_{ph}. \tag{3.85}$$

The second of the above equations can be rewritten into

$$\langle \mathrm{HF}| \, \hat{a}^\dagger_h \hat{a}_p [\hat{H}, \hat{Q}_\omega] \, |\mathrm{HF}\rangle^* = E^{\mathrm{RPA}}_\omega Y^\omega_{ph}. \tag{3.86}$$

Summarizing, we end up with

$$\langle \mathrm{HF}| \, \hat{a}^\dagger_h \hat{a}_p [\hat{H}, \hat{Q}^\dagger_\omega] \, |\mathrm{HF}\rangle \quad = E^{\mathrm{RPA}}_\omega X^\omega_{ph}, \tag{3.87}$$

$$\langle \mathrm{HF}| \, \hat{a}^\dagger_h \hat{a}_p [\hat{H}, \hat{Q}_\omega] \, |\mathrm{HF}\rangle^* = E^{\mathrm{RPA}}_\omega Y^\omega_{ph}. \tag{3.88}$$

Inserting the definition of the ECO (3.54) into the left-hand sides of the above equations leads to

$$\sum_{p'h'} \Big(X^\omega_{p'h'} \underbrace{\langle \mathrm{HF}| \, \hat{a}^\dagger_h \hat{a}_p [\hat{H}, \hat{a}^\dagger_{p'} \hat{a}_{h'}] \, |\mathrm{HF}\rangle}_{\equiv A_{ph,p'h'}} - Y^\omega_{p'h'} \underbrace{\langle \mathrm{HF}| \, \hat{a}^\dagger_h \hat{a}_p [\hat{H}, \hat{a}^\dagger_{h'} \hat{a}_{p'}] \, |\mathrm{HF}\rangle}_{\equiv -B_{ph,p'h'}} \Big) \quad = E^{\mathrm{RPA}}_\omega X^\omega_{ph}, \tag{3.89}$$

$$\sum_{p'h'} \Big(X^\omega_{p'h'}{}^* \underbrace{\langle \mathrm{HF}| \, \hat{a}^\dagger_h \hat{a}_p [\hat{H}, \hat{a}^\dagger_{h'} \hat{a}_{p'}] \, |\mathrm{HF}\rangle}_{= -B_{ph,p'h'}} - Y^\omega_{p'h'}{}^* \underbrace{\langle \mathrm{HF}| \, \hat{a}^\dagger_h \hat{a}_p [\hat{H}, \hat{a}^\dagger_{p'} \hat{a}_{h'}] \, |\mathrm{HF}\rangle}_{= A_{ph,p'h'}} \Big)^* = E^{\mathrm{RPA}}_\omega Y^\omega_{ph}, \tag{3.90}$$

or in short notation

$$\sum_{p'h'} \Big(\quad X^\omega_{p'h'} \, A_{ph,p'h'} + Y^\omega_{p'h'} \, B_{ph,p'h'} \Big) = E^{\mathrm{RPA}}_\omega X^\omega_{ph}, \tag{3.91}$$

$$\sum_{p'h'} \Big(-X^\omega_{p'h'} \, B^*_{ph,p'h'} - Y^\omega_{p'h'} \, A^*_{ph,p'h'} \Big) = E^{\mathrm{RPA}}_\omega Y^\omega_{ph}. \tag{3.92}$$

In (3.89) we have introduced two new matrices, A and B, with their matrix elements defined via

$$\boxed{A_{ph,p'h'} = \quad \langle \mathrm{HF}| \, \hat{a}^\dagger_h \hat{a}_p [\hat{H}, \hat{a}^\dagger_{p'} \hat{a}_{h'}] \, |\mathrm{HF}\rangle \, ,} \tag{3.93}$$

$$\boxed{B_{ph,p'h'} = -\langle \mathrm{HF}| \, \hat{a}^\dagger_h \hat{a}_p [\hat{H}, \hat{a}^\dagger_{h'} \hat{a}_{p'}] \, |\mathrm{HF}\rangle \, .} \tag{3.94}$$

This notation, in which we explicitly denote the individual particle (p, p') and hole (h, h') indices, is somewhat lengthy. To make things more tractable, we introduce a matrix-notation with collective-indices $i = (ph)$ and $j = (p'h')$. With this the above equations read

$$\sum_j \Big(\quad A_{i,j} X^\omega_j + B_{i,j} Y^\omega_j \Big) = E^{\mathrm{RPA}}_\omega X^\omega_i, \tag{3.95}$$

$$\sum_j \Big(-B^*_{i,j} X^\omega_j - A^*_{i,j} Y^\omega_j \Big) = E^{\mathrm{RPA}}_\omega Y^\omega_i. \tag{3.96}$$

We see that the RPA equations (3.89) and (3.90) can be written into matrix form:

$$\boxed{\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^\omega \\ Y^\omega \end{pmatrix} = E_\omega^{\mathrm{RPA}} \begin{pmatrix} X^\omega \\ Y^\omega \end{pmatrix}.} \tag{3.97}$$

Equation (3.97) is called the *RPA matrix equation*. Relation (3.97) reduces the RPA problem to an eigenvalue problem, and its solution yields the RPA eigenenergies E_ω^{RPA} as well as the RPA amplitudes X_{ph}^ω and Y_{ph}^ω. It can be shown that the matrix A is Hermitian and B is symmetric, and, therefore, the so-called *RPA supermatrix*

$$R = \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \tag{3.98}$$

is non-Hermitian. A discussion regarding the ramifications of this is given in section 3.2.7.

3.2.6 Tamm-Dancoff Approximation

The Tamm-Dancoff Approximation (TDA) is, as already mentioned, a simpler ph theory than the RPA. Within the framework of the TDA, there are ph excitations, but no hp excitations. The lack of hp excitations is the defining difference between the two theories. The ECO of the TDA consequently has the following structure

$$\hat{Q}_\omega^\dagger \overset{\mathrm{TDA}}{=} \sum_{ph} X_{ph}^\omega \, \hat{a}_p^\dagger \hat{a}_h, \tag{3.99}$$

where in comparison to the ECO of the RPA (cf. (3.54)) the second term describing the hp excitations has been omitted. The disregard of the possibility of hp excitations leads to a significant simplification of the TDA as compared to the RPA: The TDA ground state, $|\mathrm{TDA}\rangle$, has to fulfill a similar condition as the RPA ground state, namely

$$\hat{Q}_\omega \, |\mathrm{TDA}\rangle = 0 \quad \forall \omega, \tag{3.100}$$

but with the difference that now (3.100) can basically be understood as $\hat{a}_h^\dagger \hat{a}_p \, |\mathrm{TDA}\rangle = 0$. However, since $\hat{a}_p \, |\mathrm{HF}\rangle = 0 \; \forall p$, we have already found a state that obeys (3.100), and ergo we have

$$|\mathrm{TDA}\rangle = |\mathrm{HF}\rangle \, . \tag{3.101}$$

Furthermore, the TDA can be recovered from the RPA. Since there are no hp excitations (cf. (3.99)), there is no need for the Y_{ph}^ω amplitudes. Additionally, there is no B matrix, which originated from the hp part of the RPA excitation creation operator (cf. (3.62) and (3.63)). Apart from these modifications, the derivation of the TDA equations is very similar to the case of the RPA, and the TDA eigenvalue problem reads

$$AX^\omega = E_\omega^{\mathrm{TDA}} X^\omega. \tag{3.102}$$

3.2.7 Properties of the RPA equations

In section 3.2.4, we used the variational principle to derive the RPA eigenvalue problem (3.97). In this section, we will discuss some of the properties of the solutions to the RPA problem. As stated earlier, the solution of the RPA problem yields a set of quantities, namely $(E_\omega^{\mathrm{RPA}}, X_{ph}^\omega, Y_{ph}^\omega)$.

However, from a given solution we can always construct a second one by performing the following transformation

$$\begin{pmatrix} E_\omega^{\mathrm{RPA}} \\ X^\omega \\ Y^\omega \end{pmatrix} \rightarrow \begin{pmatrix} -E_\omega^{\mathrm{RPA}*} \\ Y^{\omega *} \\ X^{\omega *} \end{pmatrix}. \tag{3.103}$$

In order to confirm that the transformation (3.103) indeed gives another solution to the RPA problem we just need to plug this new set into (3.97). This yields the following transformation of the RPA equations:

$$\begin{aligned} AX^\omega + BY^\omega &= E_\omega^{\mathrm{RPA}} X^\omega \\ -B^* X^\omega - A^* Y^\omega &= E_\omega^{\mathrm{RPA}} Y^\omega \end{aligned} \quad \rightarrow \quad \begin{aligned} AY^{\omega *} + BX^{\omega *} &= -E_\omega^{\mathrm{RPA}*} Y^{\omega *} \\ -B^* Y^{\omega *} - A^* X^{\omega *} &= -E_\omega^{\mathrm{RPA}*} X^{\omega *} \end{aligned} \tag{3.104}$$

From (3.104) we see that the first transformed equation is simply the complex conjugate of the second untransformed equation. Similarly, the second transformed equation relates to the first untransformed equation. However, if we assume the original solution to have a positive energy ($E_\omega^{\mathrm{RPA}} > 0$), the new, transformed solution from (3.103) is unphysical due to the negative excitation energy ($E_\omega^{\mathrm{RPA}\prime} = -E_\omega^{\mathrm{RPA}} < 0$). Considering the form of (3.97), it is not astonishing that we get redundant solutions. We see that the RPA matrix has a block structure consisting of A and B. If n is the number of ph excitations, then both these matrices are $n \times n$ matrices and the supermatrix R is of dimension $(2n) \times (2n)$. Nevertheless, the block structure of R implies that, since no "new" information enters this matrix in the second row, some of the eigenvalues might be redundant. Under certain conditions, a reduction of the RPA eigenvalue problem to dimension n is possible [Pap07; UR71; Ull72].

In section 3.2.4 it was stated that the RPA supermatrix R is non-Hermitian. The lack of Hermiticity, of course, also allows for unphysical, complex eigenvalues. It can be shown [Tho60] that the occurrence of complex eigenvalues results from the failure of the approximate ground state to minimize the energy. In these cases, according to Thouless, the HF state is too far removed from the true ground state to be an adequate approximation. If a nucleus possesses strong ground-state deformations, which cannot be represented by Slater-determinants, then calculating excitations associated with deformations, such as quadrupole states, enlarges the model space towards deformations and suddenly the stationary condition of the variational principle is met rather by a saddle point or even a maximum than by the energy minimum, and ergo the HF state becomes unstable.

Another issue concerning the solutions of the RPA eigenvalue problem are spurious center-of-mass (CM) excitations. As long as we are dealing with closed-subshell nuclei, there is only one non-degenerate ground state, and consequently excitations with zero excitation energy should not occur. This should at least hold true in the case that the Hamiltonian is translationally invariant. Due to the fact that the calculations are always carried out with some sort of localized wave function, the conservation of the CM momentum, and with it the translational invariance, is lost. Nevertheless, it has been shown [Row70; Tho61] that the first-order RPA, when performed consistently, i.e., using the same Hamiltonian as for the HF calculation, eliminates those spurious CM excitations with exactly zero energy.

Finally, we want to give a brief remark on the RPA ground state. It can be written as (cf. [RS80])

$$|\mathrm{RPA}\rangle = N_0 \exp\left(\frac{1}{2} \sum_{ph,p'h'} Z_{ph,p'h'}\, \hat{a}_p^\dagger \hat{a}_h \hat{a}_{p'}^\dagger \hat{a}_{h'} \right) |\mathrm{HF}\rangle\,, \tag{3.105}$$

with

$$\sum_{ph} X^{\omega *}_{ph} Z_{ph,p'h'} = Y^{\omega *}_{p'h'}, \quad \forall \omega. \tag{3.106}$$

From (3.105) and (3.106) we can see that $|\mathrm{RPA}\rangle$ indeed depends on the ECOs via their amplitudes X^{ω}_{ph} and Y^{ω}_{ph}, as was stated in section 3.2.2. In matrix notation this reads

$$\sum_{i} X^{\omega *}_{i} Z_{i,j} = Y^{\omega *}_{j}, \tag{3.107}$$

which is the matrix-vector product $X^{\omega *} Z = Y^{\omega *}$. Using the entire set of vectors X^{ω} and Y^{ω} we can build matrices X and Y with the single vectors as column entries. The amplitudes Z can then be obtained as $Z = (Y X^{-1})^*$.

We can see that $|\mathrm{RPA}\rangle$ has a complicated structure, but fortunately there is no need for an actual calculation of $|\mathrm{RPA}\rangle$, since we are using the EOM approach to the RPA.

3.2.8 RPA with explicit 3B Interaction

In this section the RPA equations (3.93) and (3.94) will be evaluated for a Hamiltonian with explicit 3B forces. We will see that equations resulting from explicit 3B forces are identical to the corresponding equations within an NO2B approximation, cf. section 3.2.10. We first need the Hamiltonian $\hat{H}$ for the system under consideration. In this case, a Hamiltonian with a kinetic energy $\hat{T}$, a 2B interaction $\hat{V}$ and a 3B interaction $\hat{V}_{3\mathrm{N}}$ will be examined,

$$\hat{H} = \hat{T} + \hat{V} + \hat{V}_{3\mathrm{N}} \tag{3.108}$$

$$= \sum_{i,i'} t_{i,i'}\, \hat{a}^\dagger_i \hat{a}_{i'} + \frac{1}{4} \sum_{ij,i'j'} v_{ij,i'j'}\, \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}_{j'} \hat{a}_{i'} + \frac{1}{36} \sum_{ijk,i'j'k'} v^{3\mathrm{N}}_{ijk,i'j'k'}\, \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}^\dagger_k \hat{a}_{k'} \hat{a}_{j'} \hat{a}_{i'}. \tag{3.109}$$

In order to compute the A and B matrices, we first need to evaluate the commutator of the Hamiltonian $\hat{H}$ and pairs of creation and annihilation operators (c.f. (3.93), (3.94)), i.e., terms of the sort $[\hat{H}, \hat{a}^\dagger_{p'} \hat{a}_{h'}]$. Since

$$[\hat{H}, \hat{a}^\dagger_{p'} \hat{a}_{h'}] = [\hat{T} + \hat{V} + \hat{V}_{3\mathrm{N}}, \hat{a}^\dagger_{p'} \hat{a}_{h'}] \tag{3.110}$$

$$= [\hat{T}, \hat{a}^\dagger_{p'} \hat{a}_{h'}] + [\hat{V}, \hat{a}^\dagger_{p'} \hat{a}_{h'}] + [\hat{V}_{3\mathrm{N}}, \hat{a}^\dagger_{p'} \hat{a}_{h'}], \tag{3.111}$$

one first needs to calculate the commutators of $\hat{T}$, $\hat{V}$ and $\hat{V}_{3\mathrm{N}}$ with the term $\hat{a}^\dagger_{p'} \hat{a}_{h'}$. It is helpful to first evaluate all the basic commutators $[\hat{a}^\dagger_i, \hat{a}_j]$ that will be needed during the calculation of the above commutators. With this, we can start the actual task by evaluating the commutator involving $\hat{T}$

$$[\hat{T}, \hat{a}^\dagger_{p'} \hat{a}_{h'}] = \sum_{i,i'} t_{i,i'} [\hat{a}^\dagger_i \hat{a}_{i'}, \hat{a}^\dagger_{p'} \hat{a}_{h'}] \tag{3.112}$$

$$= \sum_{i,i'} t_{i,i'} \left(\hat{a}^\dagger_i [\hat{a}_{i'}, \hat{a}^\dagger_{p'} \hat{a}_{h'}] + [\hat{a}^\dagger_i, \hat{a}^\dagger_{p'} \hat{a}_{h'}] \hat{a}_{i'} \right) \tag{3.113}$$

$$= \sum_{i,i'} t_{i,i'} \left(\hat{a}^\dagger_i \hat{a}^\dagger_{p'} [\hat{a}_{i'}, \hat{a}_{h'}] + \hat{a}^\dagger_i [\hat{a}_{i'}, \hat{a}^\dagger_{p'}] \hat{a}_{h'} + \hat{a}^\dagger_{p'} [\hat{a}^\dagger_i, \hat{a}_{h'}] \hat{a}_{i'} + [\hat{a}^\dagger_i, \hat{a}^\dagger_{p'}] \hat{a}_{h'} \hat{a}_{i'} \right) \tag{3.114}$$

$$= \sum_{i} \left(t_{i,p'}\, \hat{a}^\dagger_i \hat{a}_{h'} - t_{h',i}\, \hat{a}^\dagger_{p'} \hat{a}_i \right). \tag{3.115}$$