Chapter 2

RPA

In this chapter, we outline the random phase approximation (RPA). In the RPA, 1-particle 1-hole excitations and collective excitations are described. Furthermore, the ground state correlations and the collective mass are considered. The RPA is valid for the description of a vibrational mode such as a giant resonance of nuclei. In section 2.1, the RPA equations in the standard particle-hole configuration space are explained (cf. [46, 47, 48]). In section 2.2, the RPA equations in mixed configuration space of coordinates and hole orbitals are introduced and the relation between the particle-hole configuration space formalism and the mixed configuration space formalism is explained. In section 2.3, we study the relation between RPA in the mixed configuration space and time-dependent Hartree-Fock (TDHF) in coordinate representation. We derive relations among the single-particle density matrices under the time-reversal operation. We also derive a relation of time reversal pair in the RPA wave function.

2.1 RPA in particle-hole configuration space

2.1.1 X-Y representation

Here we derive RPA equations starting with equations of motion method [46] (See [47]). Using hamiltonian H and phonon operators O_λ, equations of motion for the operators $O_\lambda^\dagger$ are

$$[H, O_\lambda^\dagger]|0\rangle = (E_\lambda - E_0)O_\lambda^\dagger|0\rangle = \hbar\omega_\lambda O_\lambda^\dagger|0\rangle, \tag{2.1}$$

where $|0\rangle$ is a ground state defined by

$$O_\lambda|0\rangle = 0, \tag{2.2}$$

and E_λ ($\hbar\omega_\lambda$) is the energy (the excitation energy) for excited state $|\lambda\rangle$ defined by

$$|\lambda\rangle = O_\lambda^\dagger|0\rangle. \tag{2.3}$$

Acting an arbitrary state $\langle 0|\delta O$ on Eq. (2.1) from the left and making use of the fact $\langle 0|[H, O_\lambda^\dagger] = 0$, we get

$$\langle 0|[\delta O, [H, O_\lambda^\dagger]]|0\rangle = \hbar\omega_\lambda \langle 0|[\delta O, O_\lambda^\dagger]|0\rangle. \tag{2.4}$$

We use an approximation

$$|0\rangle \simeq |\mathrm{HF}\rangle, \tag{2.5}$$

where $|\mathrm{HF}\rangle$ is Hartree-Fock ground state. We approximate an phonon operator as

$$O_\lambda^\dagger = \sum_{mi} X_{mi}^\lambda a_m^\dagger a_i - Y_{mi}^\lambda a_i^\dagger a_m, \tag{2.6}$$

where $a_m^\dagger$ is creation operator of unoccupied (particle) state and a_i is annihilation operator of occupied (hole) state. The indices i and j stand for the occupied (hole) states in HF basis and indices m and n stand for the unoccupied (particle) states. X_{mi}^λ and Y_{mi}^λ are RPA amplitudes which are determined below. The arbitrary operator δO belongs to a space spanned by the set of particle-hole $a_m^\dagger a_i$ and hole-particle $a_i^\dagger a_m$ operators. Putting Eq. (2.5) and Eq. (2.6) into Eq. (2.4), we have RPA equations in particle-hole configuration space

$$\begin{aligned} \sum_{nj} A_{minj} X_{nj}^\lambda + B_{minj} Y_{nj}^\lambda &= \hbar\omega_\lambda X_{mi}^\lambda, \\ \sum_{nj} B_{minj}^* X_{nj}^\lambda + A_{minj}^* Y_{nj}^\lambda &= -\hbar\omega_\lambda Y_{mi}^\lambda, \end{aligned} \tag{2.7}$$

where $\hbar\omega_\lambda$ is the excitation energy of RPA mode λ. We will also use indices k and l to indicate any state of HF basis. Matrices A_{minj} and B_{minj} are defined as

$$\begin{aligned} A_{minj} &= \langle \mathrm{HF}|[a_i^\dagger a_m, [H, a_n^\dagger a_j]]|\mathrm{HF}\rangle, \\ B_{minj} &= -\langle \mathrm{HF}|[a_i^\dagger a_m, [H, a_j^\dagger a_n]]|\mathrm{HF}\rangle. \end{aligned} \tag{2.8}$$

In the case of the density dependent interaction such as Skyrme interaction, matrices A_{minj} and B_{minj} take the following forms [19]:

$$\begin{aligned} A_{minj} &= (e_m - e_i)\delta_{mn}\delta_{ij} + \frac{\delta^2 E}{\delta\rho_{im}\delta\rho_{nj}}, \\ B_{minj} &= \frac{\delta^2 E}{\delta\rho_{im}\delta\rho_{jn}}, \end{aligned} \tag{2.9}$$

where $E[\rho]$ is HF energy and is considered as a functional of the single particle density matrix ρ. e_m (e_i) is single-particle energy of particle (hole) state. We write Eq. (2.7) in a matrix form:

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix}_\lambda = \hbar\omega_\lambda \begin{pmatrix} X \\ Y \end{pmatrix}_\lambda . \tag{2.10}$$

This is an eigenvalue equation for non-Hermitian matrix because matrix A is Hermitian and matrix B is symmetric. Though eigenvalues of non-Hermitian matrix may be generally complex number, we can only consider the case of real eigenvalues. This is fbecause, in the case of HF local minimum, eigenvalues of stability matrix are vanishing or positive, and then eigenvalues of RPA matrix are all real [49]. In this subsection, we assume that $\hbar\omega_\lambda$ is real and positive. In the following subsections, we consider the case with vanishing and pure imaginary eigenvalues.

From complex conjugation of Eq. (2.10), we have also

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} Y^* \\ X^* \end{pmatrix}_\lambda = -\hbar\omega_\lambda \begin{pmatrix} Y^* \\ X^* \end{pmatrix}_\lambda . \tag{2.11}$$

Therefore we consider that $\begin{pmatrix} X \\ Y \end{pmatrix}_\lambda$ is an eigenvector with positive eigenvalue $\hbar\omega_\lambda$ and $\begin{pmatrix} Y^* \\ X^* \end{pmatrix}_\lambda$ is an eigenvector with negative eigenvalue $-\hbar\omega_\lambda$.

We assume the following orthogonalization among the operators $O_\lambda^\dagger$ and O_λ.

$$\langle \mathrm{HF}|[O_\kappa, O_\lambda^\dagger]|\mathrm{HF}\rangle = \delta_{\kappa\lambda}, \tag{2.12a}$$

$$\langle \mathrm{HF}|[O_\kappa, O_\lambda]|\mathrm{HF}\rangle = \langle \mathrm{HF}|[O_\kappa^\dagger, O_\lambda^\dagger]|\mathrm{HF}\rangle = 0. \tag{2.12b}$$

Then, orthonormalization relations of the eigenvectors of RPA equations are given as follows:

$$\begin{pmatrix} X^* & Y^* \end{pmatrix}_\kappa \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix}_\lambda = \sum_{mi} [X_{mi}^{\kappa *} X_{mi}^\lambda - Y_{mi}^{\kappa *} Y_{mi}^\lambda] = \delta_{\kappa\lambda}, \tag{2.13a}$$

$$\begin{pmatrix} Y & X \end{pmatrix}_\kappa \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} Y^* \\ X^* \end{pmatrix}_\lambda = \sum_{mi} [Y_{mi}^{\kappa} Y_{mi}^{\lambda *} - X_{mi}^{\kappa} X_{mi}^{\lambda *}] = -\delta_{\kappa\lambda}, \tag{2.13b}$$

$$\begin{pmatrix} Y & X \end{pmatrix}_\kappa \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix}_\lambda = \sum_{mi} [Y_{mi}^{\kappa} X_{mi}^{\lambda} - X_{mi}^{\kappa} Y_{mi}^{\lambda}] = 0. \tag{2.13c}$$

The matrix elements for a Hermitian one-body operator F are given by

$$\langle 0|F|\lambda\rangle = \sum_{mi} F_{im} X^{\lambda}_{mi} + F_{mi} Y^{\lambda}_{mi}. \tag{2.14}$$

This equation is necessary for the calculation of the reduced transition probabilities.

2.1.2 P-Q representation

In this subsection, with the aim of dealing with vanishing eigenvalues of RPA equations, we introduce P-Q representation [46, 47]. We introduce a set of hermitian operators $\mathcal{Q}_\lambda$ and $\mathcal{P}_\lambda$ in terms of the phonon operators $O^\dagger_\lambda$ and O_λ in Eq. (2.6)

$$\mathcal{Q}_\lambda = \sqrt{\frac{\hbar}{2M_\lambda \omega_\lambda}} \left(O_\lambda + O^\dagger_\lambda\right), \tag{2.15a}$$

$$\mathcal{P}_\lambda = \frac{\hbar}{i}\sqrt{\frac{M_\lambda \omega_\lambda}{2\hbar}} \left(O_\lambda - O^\dagger_\lambda\right), \tag{2.15b}$$

where ω_λ and M_λ are positive. Then, Eq. (2.4) is replaced by the corresponding equations

$$\langle \mathrm{HF}|[\delta O, [H, \mathcal{Q}_\lambda]]|\mathrm{HF}\rangle = -\frac{i\hbar}{M_\lambda}\langle \mathrm{HF}|[\delta O, \mathcal{P}_\lambda]|\mathrm{HF}\rangle, \tag{2.16a}$$

$$\langle \mathrm{HF}|[\delta O, [H, \mathcal{P}_\lambda]]|\mathrm{HF}\rangle = i\hbar\omega^2_\lambda M_\lambda \langle \mathrm{HF}|[\delta O, \mathcal{Q}_\lambda]|\mathrm{HF}\rangle. \tag{2.16b}$$

From the expression in Eq. (2.6) and Eq. (2.15), we have

$$\mathcal{Q}_\lambda = \sum_{mi} Q^{\lambda}_{mi} a^\dagger_m a_i + Q^{\lambda *}_{mi} a^\dagger_i a_m, \tag{2.17a}$$

$$\mathcal{P}_\lambda = \sum_{mi} P^{\lambda}_{mi} a^\dagger_m a_i + P^{\lambda *}_{mi} a^\dagger_i a_m, \tag{2.17b}$$

where the relation between $\left\{X^\lambda_{mi}, Y^\lambda_{mi}\right\}$ and $\left\{Q^\lambda_{mi}, P^\lambda_{mi}\right\}$ is given by

$$Q^{\lambda}_{mi} = \sqrt{\frac{\hbar}{2M_\lambda \omega_\lambda}} \left(X^\lambda_{mi} - Y^{\lambda *}_{mi}\right), \tag{2.18a}$$

$$P^{\lambda}_{mi} = i\hbar\sqrt{\frac{M_\lambda \omega_\lambda}{2\hbar}} \left(X^\lambda_{mi} + Y^{\lambda *}_{mi}\right). \tag{2.18b}$$

Substituting Eq. (2.17) for Eq. (2.16), we have RPA equations in the P-Q representation as coupled equations

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} P \\ -P^* \end{pmatrix}_\lambda = i\hbar\omega_\lambda^2 M_\lambda \begin{pmatrix} Q \\ Q^* \end{pmatrix}_\lambda , \tag{2.19a}$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} Q \\ -Q^* \end{pmatrix}_\lambda = \frac{\hbar}{i} \frac{1}{M_\lambda} \begin{pmatrix} P \\ P^* \end{pmatrix}_\lambda . \tag{2.19b}$$

From Eq. (2.12), expectation values of commutation relations among the operators $\mathcal{Q}$ and $\mathcal{P}$ become

$$\langle \mathrm{HF}|[\mathcal{Q}_\kappa, \mathcal{P}_\lambda]|\mathrm{HF}\rangle = i\hbar\delta_{\kappa\lambda}, \tag{2.20a}$$

$$\langle \mathrm{HF}|[\mathcal{Q}_\kappa, \mathcal{Q}_\lambda]|\mathrm{HF}\rangle = \langle \mathrm{HF}|[\mathcal{P}_\kappa, \mathcal{P}_\lambda]|\mathrm{HF}\rangle = 0. \tag{2.20b}$$

Therefore orthogonalization among the operators $\mathcal{Q}$ and $\mathcal{P}$ are

$$\begin{pmatrix} Q^* & Q \end{pmatrix}_\kappa \begin{pmatrix} P \\ -P^* \end{pmatrix}_\lambda = i\hbar\delta_{\kappa\lambda}, \tag{2.21a}$$

$$\begin{pmatrix} P^* & P \end{pmatrix}_\kappa \begin{pmatrix} P \\ -P^* \end{pmatrix}_\lambda = \begin{pmatrix} Q^* & Q \end{pmatrix}_\kappa \begin{pmatrix} Q \\ -Q^* \end{pmatrix}_\lambda = 0. \tag{2.21b}$$

Taking into account the RPA ground state correlations, we have a binding energy E_{RPA} which is shifted from the HF energy E_{HF} by a correction term [47]:

$$\begin{aligned} E_{RPA} = E_{HF} &- \sum_{\lambda,(\hbar\omega_\lambda \neq 0)} \hbar\omega_\lambda \sum_{mi} \left|Y_{mi}^\lambda\right|^2 - \sum_{\lambda,(\hbar\omega_\lambda = 0)} \frac{1}{2M_\lambda} \langle \mathrm{HF}|\mathcal{P}_\lambda^2|\mathrm{HF}\rangle \\ = E_{HF} &- \sum_{\lambda,(\hbar\omega_\lambda \neq 0)} \hbar\omega_\lambda \sum_{mi} \left|Y_{mi}^\lambda\right|^2 - \sum_{\lambda,(\hbar\omega_\lambda = 0)} \frac{1}{2M_\lambda} \sum_{mi} \left|P_{mi}^\lambda\right|^2 . \end{aligned} \tag{2.22}$$

There exist spurious modes of motion of translation for all nuclei and of rotation for deformed nuclei. The operator $\mathcal{P}$ in Eq. (2.15b) is the momentum of center of mass $\boldsymbol{P}_{\mathrm{c.m.}}$ for translation and the total angular momentum J_i for rotation around the axes perpendicular to the symmetry axis: i is x and y for nuclei whose shape has axial deformation around z-axis and i is x, y and z for triaxially-deformed nuclei.

2.1.3 Treatment of pure imaginary eigenvalues of RPA equations

We consider the case where RPA equations have pure imaginary eigenvalues. According to ref. [50], RPA equations (2.19) in the Q-P representation involve solution with both real and pure imaginary eigenvalues. We define again hermitian operators $\mathcal{P}_\lambda$ and $\mathcal{Q}_\lambda$ as

$$\mathcal{Q}_\lambda = \sqrt{\frac{\hbar}{2M_\lambda|\omega_\lambda|}} \left(O_\lambda + O_\lambda^\dagger\right), \tag{2.23a}$$

$$\mathcal{P}_\lambda = \frac{\hbar}{i}\sqrt{\frac{M_\lambda|\omega_\lambda|}{2\hbar}} \left(O_\lambda - O_\lambda^\dagger\right), \tag{2.23b}$$

where we assume that M_λ is positive. Then, Eq. (2.16) becomes

$$\langle 0|[\delta O, [H, O_\lambda^\dagger]]|0\rangle = \hbar|\omega_\lambda|\langle 0|[\delta O, O_\lambda^\dagger]|0\rangle, \qquad \omega_\lambda^2 \geq 0, \tag{2.24a}$$

$$\langle 0|[\delta O, [H, O_\lambda^\dagger]]|0\rangle = -\hbar|\omega_\lambda|\langle 0|[\delta O, O_\lambda]|0\rangle, \qquad \omega_\lambda^2 \leq 0. \tag{2.24b}$$

Eq. (2.24a) is equivalent to Eq. (2.4). Substituting Eq. (2.6) for Eq. (2.24b), we have

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix}_\lambda = \hbar|\omega_\lambda| \begin{pmatrix} Y^* \\ -X^* \end{pmatrix}_\lambda . \tag{2.25}$$

Taking complex conjugation of eq. (2.25), we have also

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} Y^* \\ X^* \end{pmatrix}_\lambda = -\hbar|\omega_\lambda| \begin{pmatrix} X \\ -Y \end{pmatrix}_\lambda . \tag{2.26}$$

Defining $\overline{X}_{mi}$ and $\overline{Y}_{mi}$ through the relations

$$\begin{aligned} X_{mi}^\lambda + Y_{mi}^{\lambda *} &= \overline{X}_{mi}^\lambda + \overline{Y}_{mi}^{\lambda *}, \\ X_{mi}^\lambda - Y_{mi}^{\lambda *} &= i\left(\overline{X}_{mi}^\lambda - \overline{Y}_{mi}^{\lambda *}\right), \end{aligned} \tag{2.27}$$

we get the equations for $\overline{X}$ and $\overline{Y}$ as

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \overline{X} \\ \overline{X}^* \end{pmatrix}_\lambda = -i\hbar|\omega_\lambda| \begin{pmatrix} \overline{X} \\ -\overline{X}^* \end{pmatrix}_\lambda , \tag{2.28a}$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \overline{Y}^* \\ \overline{Y} \end{pmatrix}_\lambda = i\hbar|\omega_\lambda| \begin{pmatrix} \overline{Y}^* \\ -\overline{Y} \end{pmatrix}_\lambda . \tag{2.28b}$$

Then, we can see that Eqs. (2.28) are RPA equations with imaginary eigenvalues $\mp i\hbar|\omega_\lambda|$.

2.1.4 Simple form of P-Q representation

We consider the case where RPA equations have real or pure imaginary eigenvalues and no vanishing eigenvalues.

In order to express the RPA equations in a simple form in P-Q representation, we rewrite relations between X-Y and P-Q as

$$\phi^{(-)\lambda}_{mi} \equiv \sqrt{\frac{2M_\lambda|\omega_\lambda|}{\hbar}} Q^\lambda_{mi} = \left(X^\lambda_{mi} - Y^{\lambda *}_{mi}\right), \tag{2.29a}$$

$$\phi^{(+)\lambda}_{mi} \equiv -\frac{i}{\hbar}\sqrt{\frac{2\hbar}{M_\lambda|\omega_\lambda|}} P^\lambda_{mi} = \left(X^\lambda_{mi} + Y^{\lambda *}_{mi}\right). \tag{2.29b}$$

Then, we rewrite RPA equations (2.19) as

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \phi^{(+)} \\ \phi^{(+)*} \end{pmatrix}_\lambda = \hbar \frac{\omega_\lambda^2}{|\omega_\lambda|} \begin{pmatrix} \phi^{(-)} \\ \phi^{(-)} \end{pmatrix}_\lambda, \tag{2.30a}$$

$$\begin{pmatrix} A & -B \\ -B^* & A^* \end{pmatrix} \begin{pmatrix} \phi^{(-)} \\ \phi^{(-)*} \end{pmatrix}_\lambda = \hbar|\omega_\lambda| \begin{pmatrix} \phi^{(+)} \\ \phi^{(+)*} \end{pmatrix}_\lambda . \tag{2.30b}$$

Note that both matrices of left-hand sides of Eq. (2.30) are hermitian. Orthonormalization relations (2.21) are rewritten as

$$\begin{pmatrix} \phi^{(-)*} & \phi^{(-)} \end{pmatrix}_\kappa \begin{pmatrix} \phi^{(+)} \\ \phi^{(+)*} \end{pmatrix}_\lambda = 2\delta_{\kappa\lambda} \tag{2.31a}$$

$$\begin{pmatrix} \phi^{(-)*} & \phi^{(-)} \end{pmatrix}_\kappa \begin{pmatrix} \phi^{(-)} \\ -\phi^{(-)*} \end{pmatrix}_\lambda = \begin{pmatrix} \phi^{(+)*} & \phi^{(+)} \end{pmatrix}_\kappa \begin{pmatrix} \phi^{(+)} \\ -\phi^{(+)*} \end{pmatrix}_\lambda = 0 \tag{2.31b}$$

2.2 RPA in coordinate and hole configuration space

2.2.1 X-Y representation

We explain the RPA equations in the mixed configuration space of coordinates and occupied orbitals, which was first derived from equations of motion method [46] in the mixed configuration space by Lemmer and Vénéroni [30].

Here, starting with the RPA equations in a particle-hole configuration space, we derive the ones in a mixed configuration space of coordinates and occupied orbitals. We define the transformation from the matrix elements A_{minj} and B_{minj} in Eq. (2.8) to a set of new quantities $A_{ij}(x,x')$ and $B_{ij}(x,x')$ as

$$\begin{aligned} A_{ij}(x,x') &= \sum_{mn} \phi_m(x) A_{minj} \phi^*_n(x'), \\ B_{ij}(x,x') &= \sum_{mn} \phi_m(x) B_{minj} \phi_n(x'), \end{aligned} \tag{2.32a}$$

and from the amplitude X^λ_{mi} and Y^λ_{mi} to $X^\lambda_i(x)$ and $Y^\lambda_i(x)$ as

$$
\begin{aligned}
X^\lambda_i(x) &= \sum_m X^\lambda_{mi}\phi_m(x), \\
Y^\lambda_i(x) &= \sum_m Y^\lambda_{mi}\phi^*_m(x).
\end{aligned}
\tag{2.32b}
$$

In Eq. (2.32), x represents a set of space coordinate $\boldsymbol{r}$, spin coordinate $\sigma = \pm\frac{1}{2}$ and isospin coordinate $\tau = \pm\frac{1}{2}$, where $\tau = +\frac{1}{2} = \mathrm{n}$ represents a neutron and $\tau = -\frac{1}{2} = \mathrm{p}$ represents a proton. We use abbreviations as $\sum_x \equiv \sum_{\sigma\tau}\int \mathrm{d}\boldsymbol{r}$ and $\delta_{xx'} \equiv \delta(\boldsymbol{r}-\boldsymbol{r}')\delta_{\sigma\sigma'}\delta_{\tau\tau'}$. The wave function $\phi_i(x)$ is a single-particle wave function in coordinate representation.

Inverse transformations of Eqs. (2.32) are

$$
\begin{aligned}
A_{minj} &= \sum_{xx'} \phi^*_m(x)A_{ij}(x,x')\phi_n(x'), \\
B_{minj} &= \sum_{xx'} \phi^*_m(x)B_{ij}(x,x')\phi^*_n(x'),
\end{aligned}
\tag{2.33a}
$$

and

$$
\begin{aligned}
X^\lambda_{mi} &= \sum_x \phi^*_m(x)X^\lambda_i(x), \\
Y^\lambda_{mi} &= \sum_x \phi_m(x)Y^\lambda_i(x).
\end{aligned}
\tag{2.33b}
$$

Substituting Eqs. (2.33) for Eq. (2.7), the RPA equations in the mixed configuration space is given as

$$
\begin{aligned}
&\sum_{jx'} A_{ij}(x,x')X^\lambda_j(x') + B_{ij}(x,x')Y^\lambda_j(x') = \hbar\omega_\lambda X^\lambda_i(x) \\
&\sum_{jx'} B^*_{ij}(x,x')X^\lambda_j(x') + A^*_{ij}(x,x')Y^\lambda_j(x') = -\hbar\omega_\lambda Y^\lambda_i(x).
\end{aligned}
\tag{2.34}
$$

Defining an operator $P(x,x')$ as

$$
P(x,x') \equiv \sum_m \phi_m(x)\phi^*_m(x') = \delta_{xx'} - \sum_i \phi_i(x)\phi^*_i(x'), \tag{2.35}
$$

which is a projection operator removing occupied (hole) states in the Hartree-Fock basis from any state, the following relations for the quantities $X_i(x)$ and $Y_i(x)$ are derived from the transformation Eq. (2.32b):

$$
\sum_{x'} P(x,x')X_i(x') = X_i(x), \tag{2.36a}
$$

$$
\sum_{x'} P^*(x,x')Y_i(x') = Y_i(x). \tag{2.36b}
$$

Similarly, there holds the following relations for the matrix elements $A_{ij}(x,x')$ and $B_{ij}(x,x')$:

$$\sum_{x''} P(x,x'')A_{ij}(x'',x') = \sum_{x''} A_{ij}(x,x'')P(x''x') = A_{ij}(x,x'), \tag{2.37a}$$

$$\sum_{x''} P(x,x'')B_{ij}(x'',x') = \sum_{x''} B_{ij}(x,x'')P^*(x''x') = B_{ij}(x,x'). \tag{2.37b}$$

Putting Eq. (2.33a) into Eq. (2.9), we obtain

$$\begin{aligned} A_{ij}(x,x') &= \sum_{x''x'''} P(x,x'')\widetilde{A}_{ij}(x'',x''')P(x''',x'), \\ B_{ij}(x,x') &= \sum_{x''x'''} P(x,x'')\widetilde{B}_{ij}(x'',x''')P^*(x''',x'), \end{aligned} \tag{2.38a}$$

where $\widetilde{A}_{ij}(x,x')$ and $\widetilde{B}_{ij}(x,x')$ are defined as

$$\begin{aligned} \widetilde{A}_{ij}(x,x') &= [h(x,x') - e_i\delta(x,x')]\,\delta_{ij} \\ &\quad + \sum_{x''x'''} \phi_i(x'')\phi_j^*(x''')\frac{\partial^2 E}{\partial\rho(x'',x)\partial\rho(x',x''')}, \\ \widetilde{B}_{ij}(x,x') &= \sum_{x''x'''} \phi_i(x'')\phi_j(x''')\frac{\partial^2 E}{\partial\rho(x'',x)\partial\rho(x''',x')}. \end{aligned} \tag{2.38b}$$

The single-particle hamiltonian $h(x,x')$ is defined in Eq. (2.53).

The orthonormalization relations for the amplitudes $X_i(x)$ and $Y_i(X)$ are

$$\sum_{ix} X_i^{\kappa*}(x)X_i^{\lambda}(x) - Y_i^{\kappa*}(x)Y_i^{\lambda}(x) = \delta_{\kappa\lambda}, \tag{2.39a}$$

$$\sum_{ix} Y_i^{\kappa}(x)X_i^{\lambda}(x) - X_i^{\kappa}(x)Y_i^{\lambda}(x) = 0. \tag{2.39b}$$

and the matrix elements of a hermitian one-body operator F is expressed as

$$\langle 0|F|\lambda\rangle = \sum_i \sum_{xx'} \phi_i^*(x)F(x,x')X_i^{\lambda}(x') + Y_i^{\lambda}(x)F(x,x')\phi_i(x'). \tag{2.40}$$

2.2.2 P-Q representation

Corresponding to subsection 2.1.2, we write down the RPA equations in the P-Q representation and the mixed space configuration of coordinate and hole orbitals

$$\sum_{jx'} A_{ij}(x,x')P_i^{\lambda}(x') - B_{ij}(x,x')P_i^{\lambda *}(x') = i\hbar\omega_\lambda^2 M_\lambda Q_i^{\lambda}(x), \tag{2.41a}$$

$$\sum_{jx'} A_{ij}(x,x')Q_i^{\lambda}(x') - B_{ij}(x,x')Q_i^{\lambda *}(x') = \frac{\hbar}{i}\frac{1}{M_\lambda}P_i^{\lambda}(x), \tag{2.41b}$$

with

$$P_i^{\lambda}(x) = \sum_m P_{mi}^{\lambda}\phi_m(x) = i\hbar\sqrt{\frac{M_\lambda\omega_\lambda}{2\hbar}}\left[X_i^{\lambda}(x) + Y_i^{\lambda *}(x)\right], \tag{2.42a}$$

$$Q_i^{\lambda}(x) = \sum_m Q_{mi}^{\lambda}\phi_m^*(x) = \sqrt{\frac{\hbar}{2M_\lambda\omega_\lambda}}\left[X_i^{\lambda}(x) - Y_i^{\lambda *}(x)\right]. \tag{2.42b}$$

Then, from Eq. (2.21), orthonormalization relations for $P_i^{\lambda}(x)$ and $Q_i^{\lambda}(x)$ are

$$\sum_{ix} Q_i^{\kappa *}(x)P_i^{\lambda}(x) - Q_i^{\kappa}(x)P_i^{\lambda *}(x) = i\hbar\delta_{\kappa\lambda}, \tag{2.43a}$$

$$\sum_{ix} P_i^{\kappa *}(x)P_i^{\lambda}(x) - P_i^{\kappa}(x)P_i^{\lambda *}(x) = 0, \tag{2.43b}$$

$$\sum_{ix} Q_i^{\kappa *}(x)Q_i^{\lambda}(x) - Q_i^{\kappa}(x)Q_i^{\lambda *}(x) = 0. \tag{2.43c}$$

The RPA ground state energy E_{RPA} in Eq. (2.22) can be written as the form in the mixed configuration space:

$$E_{RPA} = E_{HF} - \sum_{\lambda,(\hbar\omega_\lambda\neq 0)} \hbar\omega_\lambda \sum_{ix} \left|Y_i^{\lambda}(x)\right|^2 - \sum_{\lambda,(\hbar\omega_\lambda = 0)} \frac{1}{2M_\lambda}\sum_{ix}\left|P_i^{\lambda}(x)\right|^2. \tag{2.44}$$

2.2.3 RPA equations suitable for Skyrme-type interaction

With the purpose of obtaining a suitable form of RPA equations for the numerical calculations, we define the new amplitude $\phi_i^{(\pm)}(x)$ as

$$\phi_i^{(\pm)\lambda}(x) \equiv \sum_m \phi_{mi}^{(\pm)\lambda}\phi_m(x), \tag{2.45}$$

or

$$\phi_i^{(-)\lambda}(x) = \sqrt{\frac{2M_\lambda|\omega_\lambda|}{\hbar}}Q_i^{\lambda}(x) = \left(X_i^{\lambda}(x) - Y_i^{\lambda *}(x)\right), \tag{2.46a}$$

$$\phi_i^{(+)\lambda}(x) = -\frac{i}{\hbar}\sqrt{\frac{2\hbar}{M_\lambda|\omega_\lambda|}}P_i^{\lambda}(x) = \left(X_i^{\lambda}(x) + Y_i^{\lambda *}(x)\right). \tag{2.46b}$$

Then, the RPA equations (2.30) in the mixed configuration space become

$$\begin{aligned}\sum_{jx'} A_{ij}(x,x')\phi_j^{(+)\lambda}(x') + B_{ij}(x,x')\phi_j^{(+)\lambda *}(x') &= \hbar\frac{\omega_\lambda^2}{|\omega_\lambda|}\phi_i^{(-)\lambda}(x), \\ \sum_{jx'} A_{ij}(x,x')\phi_j^{(-)\lambda}(x') - B_{ij}(x,x')\phi_j^{(-)\lambda *}(x') &= |\hbar\omega_\lambda|\phi_i^{(+)\lambda}(x).\end{aligned} \tag{2.47}$$

Putting Eq. (2.38) into Eq. (2.47), assuming real eigenvalues, the RPA equations are given as

$$\sum_{x'}\left[h(x,x') - e_i\delta_{xx'}\right]\phi_i^{(\pm)\lambda}(x') + \sum_{x'x''} P(x,x')h^{(\pm)\lambda}(x',x'')\phi_i(x'') = \hbar\omega_\lambda\phi_i^{(\mp)\lambda}(x) \tag{2.48}$$

with the hamiltonian

$$h^{(\pm)\lambda}(x,x'') \equiv \sum_{x'x'''} \rho^{(\pm)\lambda}(x',x''')\frac{\delta h(x,x'')}{\delta\rho(x',x''')}, \tag{2.49}$$

where densities are defined as

$$\rho^{(\pm)\lambda}(x,x''') \equiv \sum_j \phi_j^*(x''')\phi_j^{(\pm)\lambda}(x') \pm \phi_j^{(\pm)\lambda *}(x''')\phi_j(x'). \tag{2.50}$$

The density $\rho^{(+)\lambda}$ ($\rho^{(-)\lambda}$) is the (anti-)hermitian part of the general transition density matrix $\rho^\lambda(x,x')$, which is explained next section. Similarly, the hamiltonian $h^{(+)\lambda}$ ($h^{(-)\lambda}$) is the (anti-)hermitian part of the transition hamiltonian, which is defined next section.

From Eq. (2.31), the orthonormalization relations among the RPA wave functions $\phi_i^{(\pm)\lambda}(x)$ are given by

$$\sum_{ix} \phi_i^{(-)\kappa *}(x)\phi_i^{(+)\lambda}(x) + \phi_i^{(-)\kappa}(x)\phi_i^{(+)\lambda *}(x) = 2\delta_{\kappa\lambda}, \tag{2.51a}$$

$$\sum_{ix} \phi_i^{(+)\kappa *}(x)\phi_i^{(+)\lambda}(x) + \phi_i^{(+)\kappa}(x)\phi_i^{(+)\lambda *}(x) = 0, \tag{2.51b}$$

$$\sum_{ix} \phi_i^{(-)\kappa *}(x)\phi_i^{(-)\lambda}(x) + \phi_i^{(-)\kappa}(x)\phi_i^{(-)\lambda *}(x) = 0. \tag{2.51c}$$

The RPA equations (2.48) correspond to one in Ref. [51]. The form of the RPA equations (2.48) is similar to the Hartree-Fock equation. In truth, we can directly take advantage of the Skyrme-Hartree-Fock method in grid representation. First, we can make use of the time-reversal properties of the density $\rho^{(\pm)\lambda}$ and the single-particle wave function $\phi_i^{(\pm)}(x)$ for even-even nuclei (see next section). Second, we can impose spatial symmetry in the wave function for triaxial nuclei (see section 4.2.2). So, the equation (2.48) is very suitable for numerical calculation (see section 4.2).

2.3 Time reversal in RPA

2.3.1 Relation between RPA and TDHF

Hartree-Fock equation for the single-particle wave function $\phi_i(x)$ with the single-particle energy e_i is written as [10]

$$\sum_{x'} h^{(0)}(x, x')\phi_i(x') = e_i\phi_i(x), \tag{2.52}$$

where the single-particle hamiltonian $h^{(0)}(x, x') \equiv h[\rho^{(0)}(x, x')]$ is defined as

$$h[\rho(x, x')] = \frac{\partial E[\rho]}{\partial \rho(x', x)}. \tag{2.53}$$

The energy $E[\rho]$ is the expectation value of the total hamiltonian with respect to Slater determinant constructed with the single-particle wave functions and expressed as a function of the single-particle density matrix ρ. The single-particle density matrix $\rho^{(0)}(x, x')$ for the HF ground state is defined as

$$\rho^{(0)}(x, x') = \sum_{i=1}^{A} \phi_i^*(x')\phi_i(x), \tag{2.54}$$

where A is a nucleon number.

The TDHF equation for the single-particle wave function $\psi_i(x, t)$ is written as

$$i\hbar\frac{\partial}{\partial t}\psi_i(x, t) = \sum_{x'} h(x, x', t)\psi_i(x', t), \tag{2.55}$$

with the single-particle hamiltonian $h(x, x', t) = h[\rho(x, x', t)]$. The single-particle density matrix $\rho(x, x', t)$ is defined as

$$\rho(x, x', t) = \sum_{i=1}^{A} \psi_i^*(x', t)\psi_i(x, t). \tag{2.56}$$

It is well known that the RPA equation is a small amplitude limit of the TDHF equation. The single-particle wave function $\psi_i(x, t)$ is expanded around the HF ground state solution $\phi_i(x)$ in terms of the wave function $X_i^\lambda(x)$ and $Y_i^\lambda(x)$ or $\phi_i^{(\pm)\lambda}(x)$, which is defined as Eq. (2.45) [52, 53, 29]:

$$\psi_i(x, t) = [\phi_i(x) + \varepsilon\delta\psi_i(x, t)]\, \mathrm{e}^{-ie_it/\hbar}, \tag{2.57a}$$

with

$$\delta\psi_i(x,t) = X_i^\lambda(x)\,\mathrm{e}^{-i\omega_\lambda t} + Y_i^{\lambda *}(x)\,\mathrm{e}^{i\omega_\lambda t} \tag{2.57b}$$

$$= \phi_i^{(+)\lambda}(x)\cos(\omega_\lambda t) - i\phi_i^{(-)\lambda}(x)\sin(\omega_\lambda t), \tag{2.57c}$$

where ε is small parameter.

Combining the expansion form (2.57a) with the orthogonalization relation for the single-particle wave function $\psi_i(x,t)$, the following relation is derived:

$$\sum_x \left[\delta\psi_j^*(x,t)\phi_i(x) + \phi_j^*(x)\delta\psi_i(x,t)\right] = 0 \qquad (\text{for } i \neq j). \tag{2.58}$$

In order to satisfy the relation (2.58), we demand the following condition:

$$\sum_{x'} P(x,x')\delta\psi_i(x',t) = \delta\psi_i(x,t), \tag{2.59}$$

where operator $P(x,x')$, which is defined by Eq. (2.35), is a projection operator removing hole orbitals of the HF basis from any state.

Putting Eq. (2.57a) into Eq. (2.56), the single-particle density matrix $\rho(x,x',t)$ is divided into stationary part $\rho^{(0)}(x,x')$ in Eq. (2.54) and dynamical part:

$$\rho(x,x',t) = \rho^{(0)}(x,x') + \varepsilon\delta\rho(x,x',t) + O(\varepsilon^2), \tag{2.60a}$$

where the dynamical part of the single-particle density matrix is defined as

$$\delta\rho(x,x',t) = \sum_{i=1}^{A} \phi_i^*(x')\delta\psi_i(x,t) + \delta\psi_i^*(x',t)\phi_i(x). \tag{2.60b}$$

Substituting Eq. (2.57b) and Eq. (2.57c) for Eq. (2.60b), the dynamical part of the single-particle density matrix is given as

$$\delta\rho(x,x',t) = \rho^\lambda(x,x')\,\mathrm{e}^{-i\omega_\lambda t} + \rho^{\lambda\dagger}(x,x')\,\mathrm{e}^{+i\omega_\lambda t} \tag{2.61a}$$

$$= \rho^{(+)\lambda}(x,x')\cos(\omega_\lambda t) - i\rho^{(-)\lambda}(x,x')\sin(\omega_\lambda t) \tag{2.61b}$$

with

$$\rho^\lambda(x,x') = \sum_i \phi_i^*(x')X_i^\lambda(x) + Y_i^\lambda(x')\phi_i(x), \tag{2.62a}$$

$$\rho^{(\pm)\lambda}(x,x') = \sum_i \phi_i^*(x')\phi_i^{(\pm)\lambda}(x) \pm \phi_i^{(\pm)\lambda *}(x')\phi_i(x). \tag{2.62b}$$

The density $\rho^{\lambda\dagger}$ is defined as $\rho^{\lambda\dagger}(x,x') \equiv \rho^{\lambda *}(x',x)$. The relations among ρ^{λ} and $\rho^{(\pm)}$ are given as

$$\rho^{\lambda}(x,x') = \rho^{(+)\lambda}(x,x') + \rho^{(-)\lambda}(x,x') \tag{2.63}$$

and

$$\rho^{(\pm)\lambda}(x,x') = \tfrac{1}{2}\left[\rho^{\lambda}(x,x') \pm \rho^{\lambda\dagger}(x,x')\right]. \tag{2.64}$$

We call ρ^{λ} the *general transition density matrix.* The density $\rho^{(+)\lambda}$ ($\rho^{(-)\lambda}$) is the (anti-)hermitian part of the general transition density matrix.

Putting Eq. (2.60a) into the single-particle hamiltonian $h(x,x',t)$, the single-particle hamiltonian is divided into the stationary part $h^{(0)}(x,x')$ in Eq. (2.52) and the dynamical part:

$$h(x,x',t) = h^{(0)}(x,x') + \varepsilon\delta h(x,x',t) + O(\varepsilon^2) \tag{2.65a}$$

with

$$\begin{aligned}
\delta h(x,x',t) &= \sum_{x'',x'''}\left[\frac{\partial h(x,x',t)}{\partial\rho(x'',x''',t)}\right]_{\rho=\rho^{(0)}}\delta\rho(x'',x''',t) \\
&= \sum_{x'',x'''}\frac{\partial h^{(0)}(x,x')}{\partial\rho^{(0)}(x'',x''')}\delta\rho(x'',x''',t) \\
&= \sum_{x'',x'''}\frac{\partial^2 E[\rho^{(0)}]}{\partial\rho^{(0)}(x',x)\partial\rho^{(0)}(x'',x''')}\delta\rho(x'',x''',t)
\end{aligned} \tag{2.65b}$$

Substituting Eqs. (2.61) for Eq. (2.65b), the dynamical part of the single-particle hamiltonian is given as

$$\delta h(x,x',t) = h^{\lambda}(x,x')\,\mathrm{e}^{-i\omega_\lambda t} + h^{\lambda\dagger}(x,x')\,\mathrm{e}^{+i\omega_\lambda t} \tag{2.66a}$$

$$= h^{(+)\lambda}(x,x')\cos(\omega_\lambda t) - ih^{(-)\lambda}(x,x')\sin(\omega_\lambda t) \tag{2.66b}$$

with

$$h^{\lambda}(x,x') = \sum_{x'',x'''}\frac{\partial^2 E}{\partial\rho^{(0)}(x',x)\partial\rho^{(0)}(x'',x''')}\rho^{\lambda}(x'',x'''), \tag{2.67a}$$

$$h^{(\pm)\lambda}(x,x') = \sum_{x'',x'''}\frac{\partial^2 E}{\partial\rho^{(0)}(x',x)\partial\rho^{(0)}(x'',x''')}\rho^{(\pm)\lambda}(x'',x'''). \tag{2.67b}$$

The relations among h^{λ} and $h^{(\pm)}$ are given as

$$h^{\lambda}(x,x') = h^{(+)}(x,x') + h^{(-)}(x,x') \tag{2.68}$$

and

$$h^{(\pm)}(x,x') = \tfrac{1}{2}\left[h^{\lambda}(x,x') \pm h^{\lambda\dagger}(x,x')\right]. \tag{2.69}$$

We call h^{λ} the *transition hamiltonian.* The hamiltonian $h^{(+)\lambda}$ ($h^{(-)\lambda}$) is the (anti-)hermitian part of the transition hamiltonian.

Putting Eq. (2.57a) and Eq. (2.62a) into the TDHF equation Eq. (2.55), the first order in ε of the TDHF equation is given as

$$i\hbar\frac{\partial}{\partial t}\delta\psi_i(x,t) = \sum_{x'}\left[h^{(0)}(x,x') - e_i\delta_{xx'}\right]\delta\psi_i(x',t) + \delta h(x,x',t)\phi_i^{(0)}(x'). \tag{2.70}$$

In general, the wave function $\delta\psi_i(x,t)$ in Eq. (2.70) does not satisfy the condition (2.59). So, we rewrite Eq. (2.70) as

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\delta\psi_i(x,t) = &\sum_{x'}\left[h^{(0)}(x,x') - e_i\delta_{xx'}\right]\delta\psi_i(x',t) \\ &+ \sum_{x'x''}P(x,x')\delta h(x',x'',t)\phi_i^{(0)}(x''), \end{aligned} \tag{2.71}$$

with the condition (2.59).

Putting Eq. (2.57b) and Eq. (2.66a) into Eq. (2.71), then the RPA equation for the wave function $X_i^{\lambda}(x)$ and $Y_i^{\lambda *}(x)$ is derived as

$$\begin{aligned} \hbar\omega_\lambda X_i^{\lambda}(x) = &\sum_{x'}\left[h^{(0)}(x,x') - e_i\delta_{xx'}\right]X_i^{\lambda}(x') \\ &+ \sum_{x'x''}P(x,x')h^{\lambda}(x',x'')\phi_i^{(0)}(x''), \end{aligned} \tag{2.72a}$$

$$\begin{aligned} -\hbar\omega_\lambda Y_i^{\lambda *}(x) = &\sum_{x'}\left[h^{(0)}(x,x') - e_i\delta_{xx'}\right]Y_i^{\lambda *}(x') \\ &+ \sum_{x'x''}P(x,x')h^{\lambda\dagger}(x',x'')\phi_i^{(0)}(x''), \end{aligned} \tag{2.72b}$$

with the condition

$$\sum_{x'}P(x,x')X_i^{\lambda}(x') = X_i^{\lambda}(x'), \tag{2.73a}$$

$$\sum_{x'}P(x,x')Y_i^{\lambda *}(x') = Y_i^{\lambda *}(x'). \tag{2.73b}$$

Putting Eq. (2.57c) and Eq. (2.66b) into Eq. (2.71), then the RPA equation for the wave function $\phi_i^{(\pm)\lambda}(x)$ is also derived as

$$\begin{aligned}\hbar\omega_\lambda\phi_i^{(\mp)\lambda}(x) = &\sum_{x'}\left[h^{(0)}(x,x') - e_i\delta_{xx'}\right]\phi_i^{(\pm)\lambda}(x') \\ &+\sum_{x'x''}P(x,x')h^{(\pm)\lambda}(x',x'')\phi_i(x''),\end{aligned} \tag{2.74}$$

with the condition

$$\sum_{x'}P(x,x')\phi_i^{(\pm)\lambda}(x') = \phi_i^{(\pm)\lambda}(x). \tag{2.75}$$

We can see that Eq. (2.74) is exactly equivalent with the RPA equations in Eq. (2.48).

The RPA equations are also expressed in terms of the equations of motion of the density matrix. The TDHF equation for the density matrix $\rho(x,x',t)$ is given as

$$i\hbar\frac{\partial}{\partial t}\rho(x,x',t) = [h,\rho](x,x',t), \tag{2.76}$$

where

$$[h,\rho](x,x',t) \equiv \sum_{x''}h(x,x'',t)\rho(x'',x',t) - \rho(x,x'',t)h(x'',x',t). \tag{2.77}$$

Putting Eq. (2.60a) and Eq. (2.65a) into Eq. (2.76), the first order in ε of the TDHF equation is given as

$$i\hbar\frac{\partial}{\partial t}\delta\rho(x,x',t) = [h^{(0)},\delta\rho](x,x',t) + [\delta h,\rho^{(0)}](x,x',t), \tag{2.78}$$

where

$$[h^{(0)},\delta\rho](x,x',t) \equiv \sum_{x''}h^{(0)}(x,x'')\delta\rho(x'',x',t) - \delta\rho(x,x'',t)h^{(0)}(x'',x'), \tag{2.79a}$$

$$[\delta h,\rho^{(0)}](x,x',t) \equiv \sum_{x''}\delta h(x,x'',t)\rho^{(0)}(x'',x') - \rho^{(0)}(x,x'')\delta h(x'',x',t). \tag{2.79b}$$

Putting Eq. (2.61a) and Eq. (2.66a) into Eq. (2.78), then the RPA equation for the general transition density matrix $\rho^\lambda(x,x')$ is given as

$$\hbar\omega_\lambda\rho^\lambda(x,x') = [h^{(0)},\rho^\lambda](x,x') + [h^\lambda,\rho^{(0)}](x,x'). \tag{2.80}$$

Equivalently, putting Eq. (2.61b) and Eq. (2.66b) into Eq. (2.78), then the RPA equations for the hermitian and anti-hermitian part of the general transition density matrix $\rho^{(\pm)\lambda}(x,x')$ are given as

$$\hbar\omega_\lambda \rho^{(\mp)\lambda}(x,x') = [h^{(0)},\rho^{(\pm)}](x,x') + [h^{(\pm)},\rho^{(0)}](x,x'). \tag{2.81}$$

2.3.2 Time reversal symmetry of general transition density matrix

In this and following subsections, we only consider the case for even-even nuclei.

A time-reversal state of a single-particle wave function $\phi_i(x)$ is defined as [54]

$$\phi_{\bar{i}}(\boldsymbol{r}\sigma\tau) \equiv \mathcal{T}\phi_i(\boldsymbol{r}\sigma\tau) = -2\sigma\phi_i^*(\boldsymbol{r}{-\sigma}\tau) \tag{2.82}$$

with time reversal operator $\mathcal{T}$ defined as

$$\mathcal{T} = -i\sigma_y K_0, \tag{2.83}$$

where σ_y is the y-component of Pauli spin matrix and K_0 is complex conjugation operator. Then, a time-reversal of time-depending single-particle wave function $\psi_i(x,t)$ is also written as

$$\psi_{\bar{i}}(\boldsymbol{r}\sigma\tau,t) \equiv \mathcal{T}\psi_i(\boldsymbol{r}\sigma\tau,t) = -2\sigma\psi_i^*(\boldsymbol{r}{-\sigma}\tau,t). \tag{2.84}$$

The time-reversal of Eq. (2.57a) is given as

$$\psi_{\bar{i}}(x,t) = [\phi_{\bar{i}}(x) + \delta\psi_{\bar{i}}(x,t)]\,\mathrm{e}^{ie_it/\hbar}, \tag{2.85}$$

and the time reversal of Eq. (2.57b) and Eq. (2.57c) is given as

$$\delta\psi_{\bar{i}}(x,t) = X_{\bar{i}}^\lambda(x)\,\mathrm{e}^{+i\omega_\lambda t} + Y_{\bar{i}}^{\lambda *}(x)\,\mathrm{e}^{-i\omega_\lambda t}, \tag{2.86a}$$

$$= \phi_{\bar{i}}^{(+)\lambda}(x)\cos(\omega_\lambda t) + i\phi_{\bar{i}}^{(-)\lambda}(x)\sin(\omega_\lambda t), \tag{2.86b}$$

where $X_{\bar{i}}(x) = \mathcal{T}X_i(x)$, $Y_{\bar{i}}(x) = \mathcal{T}Y_i(x)$ and $\phi_{\bar{i}}^{(\pm)\lambda}(x) = \mathcal{T}\phi_i^{(\pm)\lambda}(x)$.

The time-reversal of Eq. (2.60) is given as

$$\rho^T(x,x',t) = \rho^{(0)T}(x,x') + \varepsilon\delta\rho^T(x,x',t) + O(\varepsilon^2) \tag{2.87a}$$

with

$$\rho^T(x,x',t) = \sum_{i=1}^{A} \psi_{\bar{i}}^*(x',t)\psi_{\bar{i}}(x,t), \tag{2.87b}$$

$$\rho^{(0)T}(x,x') = \sum_{i=1}^{A} \phi_{\bar{i}}^*(x')\phi_{\bar{i}}(x), \tag{2.87c}$$

$$\delta\rho^T(x,x',t) = \sum_{i=1}^{A} \phi_{\bar{i}}^*(x')\delta\psi_{\bar{i}}(x,t) + \delta\psi_{\bar{i}}^*(x',t)\phi_{\bar{i}}(x). \tag{2.87d}$$

The time-reversal of Eq. (2.61) and Eq. (2.62) is also given as

$$\delta\rho^T(x,x',t) = \rho^{\lambda T}(x,x')\,\mathrm{e}^{+i\omega_\lambda t} + \rho^{\lambda\dagger T}(x,x')\,\mathrm{e}^{-i\omega_\lambda t}, \tag{2.88a}$$

$$= \rho^{(+)\lambda T}(x,x')\cos(\omega_\lambda t) + i\rho^{(-)\lambda T}(x,x')\sin(\omega_\lambda t) \tag{2.88b}$$

with

$$\rho^{\lambda T}(x,x') = \sum_{i=1}^{A} \phi_{\bar{i}}^*(x')X_{\bar{i}}^\lambda(x) + Y_{\bar{i}}^\lambda(x')\phi_{\bar{i}}(x) \tag{2.89a}$$

$$\rho^{(\pm)\lambda T}(x,x') = \sum_{i=1}^{A} \phi_{\bar{i}}^*(x')\phi_{\bar{i}}^{(\pm)\lambda}(x) \pm \phi_{\bar{i}}^{(\pm)\lambda *}(x')\phi_{\bar{i}}(x). \tag{2.89b}$$

If the single-particle density matrix $\rho(x,x',t)$ is a dynamical solution of the TDHF equation (2.76), then the density matrix $\rho^T(x,x',-t)$ is also a solution to the TDHF equation:

$$i\hbar\frac{\partial}{\partial t}\rho^T(x,x',-t) = [h^T,\rho^T](x,x',-t), \tag{2.90}$$

where $h^T \equiv h[\rho^T]$. In terms of Eqs. (2.87a), (2.88) and (2.90), the time reversal of RPA equations for the general transition density matrix $\rho^{\lambda T}(x,x',-t)$ is given as

$$\hbar\omega_\lambda\rho^{\lambda T}(x,x') = [h^{(0)},\rho^{\lambda T}](x,x') + [h^{\lambda T},\rho^{(0)}](x,x'), \tag{2.91}$$

and for the hermitian and anti-hermitian part of the general transition density matrix $\rho^{(\pm)\lambda T}(x,x',-t)$ are given as

$$\hbar\omega_\lambda\rho^{(\mp)\lambda T}(x,x') = [h^{(0)},\rho^{(\pm)T}](x,x') + [h^{(\pm)T},\rho^{(0)}](x,x'), \tag{2.92}$$

where the relations $\rho^{(0)T} = \rho^{(0)}$ and $h^{(0)T} = h^{(0)}$ are used. Comparing Eq. (2.80) and Eq. (2.91), it is clear that, if the density matrix $\rho^\lambda(x,x')$ is the solution of the RPA equation (2.80), the density matrix $\rho^{\lambda T}(x,x')$ is also the solution of the RPA equation with same eigenvalue. Thus, there holds the relation

$$\rho^{\lambda}(x,x') = \rho^{\lambda T}(x,x'), \tag{2.93}$$

and for the hermitian and anti-hermitian part $\rho^{(\pm)}(x,x')$, the following relations hold:

$$\rho^{(\pm)\lambda}(x,x') = \rho^{(\pm)\lambda T}(x,x') \tag{2.94}$$

Furthermore, putting Eq. (2.82) for Eq. (2.87c), the relations between the single-particle density matrix and the time-reversal of that are given as

$$\rho^{(0)T}(\boldsymbol{r}\sigma\tau, \boldsymbol{r}'\sigma'\tau') = 4\sigma\sigma'\rho^{(0)*}(\boldsymbol{r}-\sigma\tau, \boldsymbol{r}'-\sigma'\tau'). \tag{2.95}$$

Similarly, the relations between the general transition density matrices and the time-reversal of those are given as

$$\rho^{\lambda T}(\boldsymbol{r}\sigma\tau, \boldsymbol{r}'\sigma'\tau') = 4\sigma\sigma'\rho^{\lambda *}(\boldsymbol{r}-\sigma\tau, \boldsymbol{r}'-\sigma'\tau'), \tag{2.96a}$$

$$\rho^{(\pm)\lambda T}(\boldsymbol{r}\sigma\tau, \boldsymbol{r}'\sigma'\tau') = 4\sigma\sigma'\rho^{(\pm)\lambda *}(\boldsymbol{r}-\sigma\tau, \boldsymbol{r}'-\sigma'\tau'). \tag{2.96b}$$

2.3.3 Time reversal property of RPA wave function

In the case of the even-even nuclei, the single-particle wave functions of HF ground state are a set of the time reversal pairs of the single-particle wave functions $\{\phi_i(x), \phi_{\bar{i}}(x); i = 1, \ldots, A/2\}$, where the subscript $\bar{i}$ indicates the time reversed states of i. Then, it is sufficient to solve the HF equation for one member of the pair. Just as in the HF case, the RPA wave functions $X_i(x)$ and $Y_i(x)$ can be made of a set of the time reversal pairs $\{X_i(x), X_{\bar{i}}(x), Y_i(x), Y_{\bar{i}}(x); i = 1, \ldots, A/2\}$. Therefore, it is sufficient to solve the RPA equations for one member of the pair. In this subsection, we derive the above relation of the time reversal pair in the RPA wave functions.

In terms of a set of the time reversal pair of the single-particle wave function $\{\phi_i, \phi_{\bar{i}}\}$, we can rewrite the general transition density in Eq. (2.62a) into

$$\begin{aligned}\rho^{\lambda}(x,x') &= \sum_{i=1}^{A/2} \left[\phi_i^*(x')X_i^{\lambda}(x) + Y_i^{\lambda}(x')\phi_i(x)\right] \\ &+ \sum_{i=1}^{A/2} \left[\phi_{\bar{i}}^*(x')X_{i+A/2}^{\lambda}(x) + Y_{i+A/2}^{\lambda}(x')\phi_{\bar{i}}(x)\right]\end{aligned} \tag{2.97}$$

and the time reversal of the general transition density matrix in Eq. (2.89a) into

$$\rho^{\lambda T}(x,x') = \sum_{i=1}^{A/2}\left[\phi_{\bar{i}}^*(x')X_{\bar{i}}^{\lambda}(x) + Y_{\bar{i}}^{\lambda}(x')\phi_{\bar{i}}(x)\right] - \sum_{i=1}^{A/2}\left[\phi_i^*(x')X_{\overline{i+A/2}}^{\lambda}(x) + Y_{\overline{i+A/2}}^{\lambda}(x')\phi_i(x)\right]. \tag{2.98}$$

Comparing ρ^{λ} with $\rho^{\lambda T}$ in terms of the Eq. (2.93), we can suppose the following relations:

$$X_{i+A/2}^{\lambda}(x) = X_{\bar{i}}^{\lambda}(x), \quad Y_{i+A/2}^{\lambda}(x) = Y_{\bar{i}}^{\lambda}(x), \qquad i = 1,\dots,A/2. \tag{2.99}$$

We confirm the above relation in terms of the RPA equation (2.34). We rewrite the RPA equation (2.34) as the matrix form

$$\begin{pmatrix} A_1 & A_2 & B_1 & B_2 \\ A_3 & A_4 & B_3 & B_4 \\ B_1^* & B_2^* & A_1^* & A_2^* \\ B_3^* & B_4^* & A_3^* & A_4^* \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ Y_1 \\ Y_2 \end{pmatrix}_{\lambda} = \hbar\omega_{\lambda} \begin{pmatrix} X_1 \\ X_2 \\ -Y_1 \\ -Y_2 \end{pmatrix}_{\lambda} \tag{2.100}$$

with

$$\begin{aligned} &\{A_1\}_{ij} = A_{ij}, && \{A_2\}_{ij} = A_{i\bar{j}}, && \{A_3\}_{ij} = A_{\bar{i}j}, && \{A_4\}_{ij} = A_{\bar{i}\bar{j}} \\ &\{B_1\}_{ij} = B_{ij}, && \{B_2\}_{ij} = B_{i\bar{j}}, && \{B_3\}_{ij} = B_{\bar{i}j}, && \{B_4\}_{ij} = B_{\bar{i}\bar{j}} \\ &\{X_1\}_i = X_i^{\lambda}, && \{X_2\}_i = X_{i+A/2}^{\lambda}, && \{Y_1\}_i = Y_i^{\lambda}, && \{Y_2\}_i = Y_{i+A/2}^{\lambda}, \end{aligned}$$

where i, j run over from 1 to $A/2$ and coordinates x, x' is omitted. Now, time reversed equations of the RPA equations is written as

$$\begin{pmatrix} A_4 & -A_3 & B_4 & -B_3 \\ -A_2 & A_1 & -B_2 & B_1 \\ B_4^* & -B_3^* & A_4^* & -A_3^* \\ -B_2^* & B_1^* & -A_2^* & A_1^* \end{pmatrix} \begin{pmatrix} \mathcal{T}X_1 \\ \mathcal{T}X_2 \\ \mathcal{T}Y_1 \\ \mathcal{T}Y_2 \end{pmatrix}_{\lambda} = \hbar\omega \begin{pmatrix} \mathcal{T}X_1 \\ \mathcal{T}X_2 \\ -\mathcal{T}Y_1 \\ -\mathcal{T}Y_2 \end{pmatrix}_{\lambda}, \tag{2.101}$$

where we use transformation $\mathcal{T}\{\phi_i, \phi_{\bar{i}}\} \to \{\phi_{\bar{i}}, -\phi_i\}$. Replacing the column matrices and the row matrices appropriately, we can rewrite above equation into

$$\begin{pmatrix} A_1 & A_2 & B_1 & B_2 \\ A_3 & A_4 & B_3 & B_4 \\ B_1^* & B_2^* & A_1^* & A_2^* \\ B_3^* & B_4^* & A_3^* & A_4^* \end{pmatrix} \begin{pmatrix} -\mathcal{T}X_2 \\ \mathcal{T}X_1 \\ -\mathcal{T}Y_2 \\ \mathcal{T}Y_1 \end{pmatrix}_{\lambda} = \hbar\omega \begin{pmatrix} -\mathcal{T}X_2 \\ \mathcal{T}X_1 \\ \mathcal{T}Y_2 \\ -\mathcal{T}Y_1 \end{pmatrix}_{\lambda}. \tag{2.102}$$

If the eigenvalues is not degenerate, then

$$\begin{pmatrix} X_1 \\ X_2 \\ Y_1 \\ Y_2 \end{pmatrix}_\lambda = a \begin{pmatrix} -\mathcal{T}X_2 \\ \mathcal{T}X_1 \\ -\mathcal{T}Y_2 \\ \mathcal{T}Y_1 \end{pmatrix}_\lambda . \tag{2.103}$$

Thus, we can obtain the relation in Eq. (2.99) when $a = 1$. Finally, we can write down the RPA wave function as

$$\begin{pmatrix} X_1 \\ X_2 \\ Y_1 \\ Y_2 \end{pmatrix}_\lambda = \begin{pmatrix} X_1 \\ \mathcal{T}X_1 \\ Y_1 \\ \mathcal{T}Y_1 \end{pmatrix}_\lambda . \tag{2.104}$$

We can use (2.104) for the case where eigenvalues are degenerate: If there are m-fold degenerate solutions of Eq. (2.100), it is clear that there are also the m-fold degenerate solutions of Eq. (2.102). We simply write down each solutions as $\boldsymbol{x}_i$ and $\boldsymbol{y}_i$ respectively. Then, the vector $\boldsymbol{y}_i$ can be transformed into the vector $\boldsymbol{x}_i$ under the following transformation:

$$\boldsymbol{x}_i = \sum_{j=1}^{m} T_{ij}\boldsymbol{y}_j, \qquad j = 1, \ldots, m. \tag{2.105}$$

We diagonalize the matrix T:

$$T = U^\dagger \widetilde{T} U, \tag{2.106}$$

where U is unitary matrix and $\widetilde{T}$ is diagonal matrix. We define new vectors as

$$\tilde{\boldsymbol{x}}_i = \sqrt{\widetilde{T}_{ii}} \sum_{j=1}^{m} U_{ij}\boldsymbol{x}_j, \quad \tilde{\boldsymbol{y}}_i = \sqrt{\widetilde{T}_{ii}} \sum_{j=1}^{m} U_{ij}\boldsymbol{y}_j, \qquad j = 1, \ldots, m. \tag{2.107}$$

Therefore, we obtain the relation

$$\tilde{\boldsymbol{x}}_i = \tilde{\boldsymbol{y}}_i, \qquad j = 1, \ldots, m. \tag{2.108}$$