Note for HFB and QRPA applied to collective excitations

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The quasiparticle random-phase approximation (QRPA), within a framework of the nuclear energy density functional (EDF) theory, has been a standard tool to access the collective excitations of atomic nuclei. For an efficient solution of this QRPA problem, finite-amplitude method (FAM) was developed.

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I. CONVENTION

Conjugation: as our convention,

$$x^* \cdots \text{ complex conjugate of the scalar } x,$$
$$\hat{\mathcal{X}}^\dagger \cdots \text{ Hermite conjugate of the operator } \hat{\mathcal{X}}. \qquad (1)$$

Note that the Hermite conjugate will be applied also to the matrix quantities.

Particle operators: in this note, the original and quasi-particle (QP) operators are represented as

$$c_k^\dagger \ \& \ c_k \cdots \text{ Original creation \& annihilation,}$$
$$a_k^\dagger \ \& \ a_k \cdots \text{ QP creation \& annihilation.}$$

Of course, $\left\{c_k^\dagger, c_l\right\} = \left\{a_k^\dagger, a_l\right\} = \delta_{kl}$ for fermions.

HEB-ground state: the state $|\Phi\rangle$ indicates so-called HFB vacuum state. Thus,

$$a_k |\Phi\rangle = 0. \qquad (2)$$

Note also that $c_k |\Phi\rangle \neq 0$ in general. To avoid the confusion, the vacuum of c_k is noted as $c_k |-\rangle = 0$ in the following. In the HFB formalism, this vacuum $|\Phi\rangle$ coincides the HFB ground state (GS) of the many-body system of interest. If the pairing correlation vanishes, the HFB GS becomes so-called HF GS: $|\Phi\rangle = |\mathrm{HF}\rangle$, where $|\mathrm{HF}\rangle = c_A^\dagger \cdots c_1^\dagger |-\rangle$.

Hamiltonian: Hamiltonian for multi-fermion systems, including up to the two-body interactions, is given as

$$\hat{\mathcal{H}} = \sum_{kl} \epsilon_{kl} c_k^\dagger c_l + \frac{1}{4} \sum_{a\neq b} \sum_{c\neq d} \tilde{v}_{ab,cd} \left(c_b c_a\right)^\dagger c_d c_c, \qquad (3)$$

in terms of the original particles. Notice that, for hermiticy $\hat{\mathcal{H}}^\dagger = \hat{\mathcal{H}}$, the coefficients ϵ_{kl} and $\tilde{v}_{ab,cd}$ must be REAL. The consistent energy-density functional $\mathcal{E}$ is determined as the expectation value of $\hat{\mathcal{H}}$ via the HFB GS. That is,

$$\mathcal{E}[\rho,\kappa,\kappa^*] = H_\Phi \equiv \left\langle \Phi \middle| \hat{\mathcal{H}} \middle| \Phi \right\rangle. \qquad (4)$$

Of course, this $\mathcal{E}$ is REAL.

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II. BASIC FORMALISM

For basic formulas of the EDF and QRPA, read also Refs. [1, 2] carefully.

A. Density matrix and pairing tensor

We start from the (relativistic) energy functional $\mathcal{E}[\rho,\kappa,\kappa^*] = \langle \Phi \mid \mathcal{H} \mid \Phi \rangle$, which is a functional of the DENSITY MATRIX and PAIRING TENSOR [2]:

$$\rho_{kl} \equiv \left\langle \Phi \mid c_l^\dagger c_k \mid \Phi \right\rangle, \qquad (5)$$
$$\Leftrightarrow \rho_{kl}^* = \left\langle \Phi \mid c_k^\dagger c_l \mid \Phi \right\rangle = \rho_{lk},$$
$$\kappa_{kl} \equiv \langle \Phi \mid c_l c_k \mid \Phi \rangle, \qquad (6)$$
$$\Leftrightarrow -\kappa_{kl}^* = \left\langle \Phi \mid c_l^\dagger c_k^\dagger \mid \Phi \right\rangle,$$

where $|\Phi\rangle$ is the HFB ground state (GS) and $c_k^\dagger$ is the creation operator of the original particle (fermion). Be careful for the opposite labels between ρ_{kl} and $c_l^\dagger c_k$ inside.

It is worthwhile to determine the density-pairing supermatrix:

$$\mathsf{R} \equiv \begin{pmatrix} \left\langle \Phi \mid c_l^\dagger c_k \mid \Phi \right\rangle & \langle \Phi \mid c_l c_k \mid \Phi \rangle \\ \left\langle \Phi \mid c_l^\dagger c_k^\dagger \mid \Phi \right\rangle & \left\langle \Phi \mid c_l c_k^\dagger \mid \Phi \right\rangle \end{pmatrix} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}. \qquad (7)$$

Indeed, this satisfies $\mathsf{R}^2 = \mathsf{R}$ in any case.

B. Quasi-particle space

Bogoliubov transformation:

$$a_k = U_{kl}^\dagger c_l + V_{kl}^\dagger c_l^\dagger$$
$$a_k^\dagger = V_{lk} c_l + U_{lk} c_l^\dagger, \qquad (8)$$

or equivalently,

$$\begin{pmatrix} a_\downarrow \\ a_\downarrow^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c_\downarrow \\ c_\downarrow^\dagger \end{pmatrix} \equiv \hat{\mathcal{W}}^\dagger \begin{pmatrix} c_\downarrow \\ c_\downarrow^\dagger \end{pmatrix}, \qquad (9)$$

where $c_a^\dagger$ (c_a) is the original s.p. creation (annihilation) operator for, e.g. the (n_a, l_a, j_a, m_a) orbit. Note also its inverse transformation:

$$\begin{pmatrix} c_\downarrow \\ c_\downarrow^\dagger \end{pmatrix} = \hat{\mathcal{W}} \begin{pmatrix} a_\downarrow \\ a_\downarrow^\dagger \end{pmatrix} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \begin{pmatrix} a_\downarrow \\ a_\downarrow^\dagger \end{pmatrix}. \tag{10}$$

This transformation must be unitary, in order to keep the anti-commutation property:

$$\hat{\mathcal{W}}^\dagger \hat{\mathcal{W}} = \hat{\mathcal{W}} \hat{\mathcal{W}}^\dagger = \mathbf{1}$$
$$\Longleftrightarrow \left\{ c_k^\dagger, c_l \right\} = \left\{ a_k^\dagger, a_l \right\} = \delta_{kl}. \tag{11}$$

Also, this transformation is determined so as to diagonalize R as

$$\hat{\mathcal{W}}^\dagger \mathsf{R} \hat{\mathcal{W}} = \begin{pmatrix} \left\langle \Phi \mid a_l^\dagger a_k \mid \Phi \right\rangle & \left\langle \Phi \mid a_l a_k \mid \Phi \right\rangle \\ \left\langle \Phi \mid a_l^\dagger a_k^\dagger \mid \Phi \right\rangle & \left\langle \Phi \mid a_l a_k^\dagger \mid \Phi \right\rangle \end{pmatrix}$$
$$= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{12}$$

This condition determines the HFB GS, $|\Phi\rangle$. In this sense, the HFB GS must be *vacuum* for $a_k^\dagger$ and a_k, except the constant shift: $a_k |\Phi\rangle = 0$. When the HFB solution is obtained in such a way, for the quasi-particle density via the HFB GS,

$$\xi_{\mu\nu} \equiv \left\langle \Phi \middle| a_\nu a_\mu^\dagger \middle| \Phi \right\rangle = \delta_{\mu\nu}. \tag{13}$$

Thus, the consistent operator must be formulated as

$$\hat{\xi} = \sum_\rho |a_\rho\rangle \langle a_\rho|, \text{ where } |a_\rho\rangle \equiv a_\rho^\dagger |\Phi\rangle, \tag{14}$$

to satisfy that $\xi_{\mu\nu} = \left\langle a_\mu \middle| \hat{\xi} \middle| a_\nu \right\rangle = \delta_{\mu\nu}$.

Matrix variables ρ_{kl} and Δ_{kl} can be now represented by the Bogoliubov matrices:

$$\rho_{kl} = \left(V^* V^T\right)_{kl}, \quad \kappa_{kl} = \left(V^* U^T\right)_{kl} = -\left(UV^\dagger\right)_{kl}. \tag{15}$$

As long as $|\Phi\rangle$ is the vacuum for the quasi particles $a_k^\dagger$ and a_l, the following identity stands:

$$\left\langle \Phi \left[a_j a_i, (a_l a_k)^\dagger \right] \Phi \right\rangle = \left\langle \Phi \mid \left\{ \left[a_i, (a_l a_k)^\dagger \right], a_j \right\} \mid \Phi \right\rangle$$
$$= \delta_{ik}\delta_{jl} - \delta_{jk}\delta_{il}, \tag{16}$$

where $\{A, B\} \equiv AB + BA$. For example, let us consider an Hermite operator $\hat{\mathcal{H}}$, which has the form

$$\hat{\mathcal{H}} = ... + \frac{1}{2} \sum_{k \neq l} H_{kl}^{20} (a_l a_k)^\dagger + \text{h.c.} + ..., \tag{17}$$

where $H_{lk}^{20} = (-) H_{kl}^{20}$ is automatically required for fermions, since $(a_k a_l)^\dagger = (-)(a_l a_k)^\dagger$. Then, the identity (16) helps to compute the expanding coefficient H_{ij}^{20}. That is

$$H_{ij}^{20} = \langle \Phi \left[a_j a_i, \mathcal{H} \right] \Phi \rangle = \langle \Phi \mid \{ [a_i, \mathcal{H}], a_j \} \mid \Phi \rangle. \tag{18}$$

Indeed,

$$RHS = \frac{1}{2} \sum_{k \neq l} \left(\delta_{ik}\delta_{jl} - \delta_{jk}\delta_{il} \right) H_{kl}^{20}$$
$$= \frac{1}{2} \left(H_{ij}^{20} - H_{ji}^{20} \right) = H_{ij}^{20}, \quad \text{Q.E.D.}$$

Similarly, for the coefficient H_{kl}^{11} for $\sum_{kl} a_k^\dagger a_l$ term, one can proof that

$$\left\langle \Phi \mid \left\{ \left[a_i, a_k^\dagger a_l \right], a_j^\dagger \right\} \mid \Phi \right\rangle = \delta_{ik}\delta_{jl}, \tag{19}$$

and thus,

$$H_{ij}^{11} = \left\langle \Phi \mid \left\{ [a_i, \mathcal{H}], a_j^\dagger \right\} \mid \Phi \right\rangle. \tag{20}$$

C. Many-body Hamiltonian

The single-particle Hamiltonian h and the pairing potential Δ are obtained as variation products of the energy functional with respect to ρ and κ, respectively:

$$h_{kl}[\rho, \kappa, \kappa^*] \equiv \frac{\partial \mathcal{E}}{\partial \rho_{lk}}, \quad \Delta_{kl}[\rho, \kappa, \kappa^*] \equiv \frac{\partial \mathcal{E}}{\partial \kappa_{kl}^*}. \tag{21}$$

Be careful for the opposite indexes of h_{kl} and ρ_{lk}. Note that $h^\dagger = h$ as well as $h^T = h^*$, consistently to that $\rho_{lk}^* = \rho_{kl}$. Also, one can formulate h and Δ in the supermatrix form:

$$\mathsf{H} \equiv \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} = \frac{\partial \mathcal{E}[\mathsf{R}]}{\partial \mathsf{R}}, \tag{22}$$

where R is giev in Eq. (7).

In order to hold the consistency to Eq. (21), the total Hamiltonian should be represented as

$$\mathcal{H} = \sum_{kl} h_{kl} c_k^\dagger c_l + \frac{1}{2} \sum_{k \neq l} \left[\Delta_{kl} c_k^\dagger c_l^\dagger + \Delta_{kl}^* c_l c_k \right] + \hat{\mathcal{N}}_\Phi [...]$$
$$+ const., \tag{23}$$

since $\mathcal{E}[\rho, \kappa, \kappa^*] = \langle \Phi \mid \mathcal{H} \mid \Phi \rangle$. Here $\hat{\mathcal{N}}_\Phi$ means the normal ordering with respect to $|\Phi\rangle$: $\left\langle \Phi \mid \hat{\mathcal{N}}_\Phi [...] \mid \Phi \right\rangle = 0$. Also, it is sometimes useful to represent the first term as

$$\sum_{kl} h_{kl} c_k^\dagger c_l = \frac{1}{2} \sum_{kl} h_{kl} c_k^\dagger c_l + \frac{1}{2} \sum_{ij} (-) h_{ij}^* c_i c_j^\dagger, \tag{24}$$

where we have utilized $h^T = h^*$.

On the other side, the original form of $\mathcal{H}$ was, of course,

$$\mathcal{H} = \sum_{kl} \epsilon_{kl} c_k^\dagger c_l + \frac{1}{4} \sum_{a \neq b} \sum_{c \neq d} \tilde{v}_{ab,cd} (c_b c_a)^\dagger c_d c_c, \tag{25}$$

in terms of the original particles. The relation between (h, Δ) and $(\epsilon, \tilde{v})$ can be indeed given as

$$h_{kl} = \epsilon_{kl} + \Gamma_{kl}, \quad \Gamma_{kl} = \sum_{pq} \tilde{v}_{kq,lp} \rho_{pq},$$
$$\Delta_{kl} = \frac{1}{2} \sum_{pq} \tilde{v}_{kl,pq} \kappa_{pq}. \tag{26}$$

The proof of this relation is from Wick's theorem. Namely, we can utilize that ρ_{kl}, κ_{kl} and $-\kappa^*_{kl}$ are nothing but *contractions* of $c_l^\dagger c_k$, $c_l c_k$ and $c_l^\dagger c_k^\dagger$ for the HFB GS $|\Phi\rangle$, respectively. Thus, for the four-point term[1],

$$\begin{aligned}(c_b c_a)^\dagger c_d c_c = \rho_{ca} c_b^\dagger c_d + \rho_{db} c_a^\dagger c_c - \rho_{da} c_b^\dagger c_c - \rho_{cb} c_a^\dagger c_d \\ -\kappa^*_{ba} c_d c_c + \kappa_{cd} c_a^\dagger c_b^\dagger \\ +\rho_{ca}\rho_{db} - \rho_{da}\rho_{cb} - \kappa^*_{ba}\kappa_{cd} \\ +\hat{\mathcal{N}}_\Phi [...] ,\end{aligned} \tag{27}$$

where $\rho\rho$ and $\kappa^*\kappa$ terms provide only a constant shift. Substituting this identity into Eq. (25) leads to Eq. (23). Note also that

$$\begin{aligned} h_{lk} &= \left\langle \Phi \mid \left\{ A_l, c_k^\dagger \right\} \mid \Phi \right\rangle, \quad A_l \equiv [c_l, \mathcal{H}], \\ \Delta_{lk} &= \langle \Phi \mid \{A_l, c_k\} \mid \Phi \rangle, \\ -\Delta^*_{lk} &= \left\langle \Phi \mid \left\{ B_l, c_k^\dagger \right\} \mid \Phi \right\rangle, \quad B_l \equiv \left[c_l^\dagger, \mathcal{H} \right], \\ -h^*_{lk} &= \langle \Phi \mid \{B_l, c_k\} \mid \Phi \rangle ,\end{aligned} \tag{28}$$

as Eq. (7.40) in Ref. [3][2]

D. Quasi-particle representation

By using the quasiparticles $a_i^\dagger$ (creation) and a_j (annihilation), the same Hamiltonian reads[3]

$$\begin{aligned}\hat{\mathcal{H}} = H_\Phi + \sum_{ij} H^{11}_{ij} a_i^\dagger a_j + \frac{1}{2}\sum_{i\neq j}\left[H^{20}_{ij} a_i^\dagger a_j^\dagger + \text{h.c.}\right] \\ +\mathcal{H}_R \left(a_*^{\dagger 4} + \text{h.c.},\ a_*^{\dagger 3} a_* + \text{h.c.},\ a_*^{\dagger 2} a_*^2 \right),\end{aligned} \tag{29}$$

where $H_\Phi \equiv \left\langle \Phi \middle| \hat{\mathcal{H}} \middle| \Phi \right\rangle$ and the residual term $\mathcal{H}_R$ contains all the four-point products. Namely,

$$\begin{aligned}\mathcal{H}_R = \sum_{ijkl}\left[H^{40}_{ijkl} a_i^\dagger a_j^\dagger a_k^\dagger a_l^\dagger + \text{h.c.} + H^{31}_{ijkl} a_i^\dagger a_j^\dagger a_k^\dagger a_l + \text{h.c.}\right] \\ +\frac{1}{4}\sum_{ab,cd} H^{22}_{ab,cd} (a_b a_a)^\dagger a_d a_c.\end{aligned} \tag{30}$$

Notice the factor 1/4 in the last term.

(i) When one takes the expectation value of $\hat{\mathcal{H}}$ via the HFB GS, it explicitly vanishes except the first term: $\left\langle \Phi \mid \hat{\mathcal{H}} - H_\Phi \mid \Phi \right\rangle = 0$. This vacuum expectation value, which is nothing but the energy functional, is given as, from Eqs. (25) and (27),

$$\begin{aligned} H_\Phi = \mathcal{E}[\rho, \kappa, \kappa^*] &= \left\langle \Phi \mid \hat{\mathcal{H}} \mid \Phi \right\rangle \\ &= \sum_{kl} \epsilon_{kl}\rho_{lk} \\ &+ \sum_{ab,cd}\left[\frac{1}{2}\rho_{ac}\tilde{v}_{ab,cd}\rho_{bd} + \frac{1}{4}\kappa^*_{ba}\tilde{v}_{ab,cd}\kappa_{dc}\right].\end{aligned} \tag{31}$$

(ii) For the coefficients H^{11}_{ij} and H^{20}_{ij} in Eq. (29), from the Bogoliubov transformation, one can find that

$$\begin{aligned} H^{11}_{ij} &= \left\{ U^\dagger h U - V^\dagger h^T V + U^\dagger \Delta V - V^\dagger \Delta^* U \right\}_{ij} \\ &= \left\{ \left(U^\dagger, V^\dagger \right) \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} \right\}_{ij},\end{aligned} \tag{32}$$

as well as,

$$\begin{aligned} H^{20}_{ij} &= \left\{ U^\dagger h V^* - V^\dagger h^T U^* + U^\dagger \Delta U^* - V^\dagger \Delta^* V^* \right\}_{ij} \\ &= \left\{ \left(U^\dagger, V^\dagger \right) \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} V^* \\ U^* \end{pmatrix} \right\}_{ij}.\end{aligned} \tag{33}$$

Remember also that, from the identities (16) and (19), those can be calculated as

$$\begin{aligned} H^{11}_{ij} &= \left\langle \Phi \mid \left\{ [a_i, \mathcal{H}], a_j^\dagger \right\} \mid \Phi \right\rangle, \\ H^{20}_{ij} &= \langle \Phi \mid \{ [a_i, \mathcal{H}], a_j \} \mid \Phi \rangle = \langle \Phi [a_j a_i, \mathcal{H}] \Phi \rangle .\end{aligned} \tag{34}$$

(iii) Now it is worthwhile to determine the supermatrices H and H' as

$$\mathsf{H} \equiv \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}, \quad \mathsf{H}' \equiv \begin{pmatrix} H^{11} & H^{20} \\ -H^{20*} & -H^{11*} \end{pmatrix}. \tag{35}$$

Thus, from Eqs. (23) and (29), the many-body Hamiltonian reads

$$\mathcal{H} = \frac{1}{2} \left(c_\rightarrow^\dagger,\ c_\rightarrow \right) \mathsf{H} \begin{pmatrix} c_\downarrow \\ c_\downarrow^\dagger \end{pmatrix} + \hat{\mathcal{N}}_\Phi [...] + const., \tag{36}$$

$$= H_\Phi + \frac{1}{2} \left(a_\rightarrow^\dagger,\ a_\rightarrow \right) \mathsf{H}' \begin{pmatrix} a_\downarrow \\ a_\downarrow^\dagger \end{pmatrix} + \mathcal{H}_R. \tag{37}$$

Because of the unitarity of the Bogoliubov transformation, $\hat{\mathcal{W}}\hat{\mathcal{W}}^\dagger = \hat{1}$, comparing the quadratic terms in both equations, one naturally concludes

$$\mathsf{H}' = \hat{\mathcal{W}}^\dagger \mathsf{H} \hat{\mathcal{W}}. \tag{38}$$

How to concretely determine the Bogoliubov transformation $\hat{\mathcal{W}}$? The answer to this question is simple: it must be determined so as to realize the vacuum state $|\Phi\rangle$ as the ground state of the Hamiltonian $\hat{\mathcal{H}}$. This condition can be satisfied by solving so-called Hartree-Fock-Bogoliubov (HFB) equation.

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[1] See Eq. (7.47) in the textbook [3].

[2] For the proof, remember that $\left[c_l, \sum_{ij} c_i^\dagger c_j h_{ij} \right] = \sum_j c_j h_{lj}$ and $\left[c_k^\dagger, \sum_{ij} c_i^\dagger c_j h_{ij} \right] = \sum_i c_i^\dagger h_{ik}$, etc.

[3] See Eq. (E.18) in Ref. [3].

III. HFB EQUATION

If the state $|\Phi\rangle$ is truly the GS of $\hat{\mathcal{H}}$, its functional derivation should be zero for an arbitrary way of the variation[4]: $|\Phi\rangle \longrightarrow |\Phi'\rangle = |\Phi\rangle + |\delta\Phi\rangle$. That is,

$$\frac{\delta \langle \Phi' \mid \mathcal{H} \mid \Phi' \rangle}{\delta \langle \Phi' \mid \Phi' \rangle} = 0. \tag{39}$$

From Thouless theorem, one can generally represent an arbitrary HFB-functional shift from the GS by using the Hermite operator,

$$\begin{aligned}\mathcal{G} &\equiv \sum_{k<l} Z_{kl} a_k^\dagger a_l^\dagger + \text{h.c.} = \sum_{k<l} Z_{kl} a_k^\dagger a_l^\dagger + \sum_{k'<l'} a_{l'} a_{k'} \left(Z_{k'l'}\right)^\dagger \\ &= \frac{1}{2}\sum_{a\neq b} \left[Z_{ab} (a_b a_a)^\dagger + (-) Z_{ab}^* (a_b a_a) \right]. \end{aligned} \tag{40}$$

Then the functional variation can be represented as[5]

$$|\Phi'\rangle = e^{i\mathcal{G}} |\Phi\rangle. \tag{41}$$

We now expand it up to the second order:

$$|\Phi'\rangle \cong \left[1 + i\mathcal{G} - \frac{\mathcal{G}^2}{2}\right] |\Phi\rangle, \quad \langle\Phi'| \cong \langle\Phi| \left[1 - i\mathcal{G} - \frac{\mathcal{G}^2}{2}\right]. \tag{42}$$

Thus, up to the second order of $\mathcal{G}$, the energy variation reads

$$\langle \Phi' \mid \mathcal{H} \mid \Phi' \rangle \cong \langle\Phi| \left(\mathcal{H} - i\left[\mathcal{G}, \mathcal{H}\right] + \frac{1}{2}\mathcal{J}\right) |\Phi_0\rangle, \tag{43}$$

where $\mathcal{J}$ is the double commutator:

$$\mathcal{J} = 2\mathcal{G}\mathcal{H}\mathcal{G} - \mathcal{H}\mathcal{G}\mathcal{G} - \mathcal{G}\mathcal{G}\mathcal{H} = \left[\mathcal{G}, \mathcal{H}\mathcal{G} - \mathcal{G}\mathcal{H}\right]. \tag{44}$$

Now we need to do some calculations:

$$\langle \Phi' \mid \mathcal{H} \mid \Phi' \rangle = H_\Phi + H_1 + H_2 + \hat{O}\left(\mathcal{G}^3\right),$$

where

$$\begin{aligned} H_1 &= \frac{-i}{2}\sum_{k\neq l} \langle\Phi| \left\{ Z_{kl}\left[(a_l a_k)^\dagger, \mathcal{H}\right] + (-) Z_{kl}^* \left[a_l a_k, \mathcal{H}\right] \right\} |\Phi\rangle, \\ H_2 &= \frac{1}{8}\sum_{k\neq l}\sum_{m\neq n} \langle\Phi| \left\{ Z_{kl}\left[(a_l a_k)^\dagger, \left[\mathcal{H}, (a_n a_m)^\dagger\right]\right] Z_{mn} \right. \\ &\qquad + Z_{kl}\left[(a_l a_k)^\dagger, \left[\mathcal{H}, a_n a_m\right]\right](-)Z_{mn}^* \\ &\quad + (-)Z_{kl}^*\left[a_l a_k, \left[\mathcal{H}, (a_n a_m)^\dagger\right]\right] Z_{mn} \\ &\quad \left. +(-)Z_{kl}^*\left[a_l a_k, \left[\mathcal{H}, a_n a_m\right]\right](-)Z_{mn}^* \right\} |\Phi\rangle. \end{aligned} \tag{45}$$

Defining the following notations,

$$G_{kl}^{20} \equiv \langle \Phi \left[a_l a_k, \mathcal{H}\right] \Phi \rangle \;\Leftrightarrow\; G_{lk}^{20*} \equiv \left\langle \Phi \left[\mathcal{H}, (a_l a_k)^\dagger\right] \Phi \right\rangle, \tag{46}$$

then the H_1 term can be represented as

$$H_1 = \frac{-i}{2}\sum_{k\neq l} \left[Z_{kl} G_{kl}^{20*} + (-) Z_{kl}^* G_{kl}^{20} \right]. \tag{47}$$

Notice that, from Eq. (34), $G^{20} = H^{20}$ and $G^{20*} = H^{20*}$, indeed.

Similarly for the H_2 term, we define[6]

$$\begin{aligned} A_{ab,cd} &\equiv \left\langle \Phi \left[a_b a_a,\ \mathcal{H} a_c^\dagger a_d^\dagger - a_c^\dagger a_d^\dagger \mathcal{H}\right] \Phi \right\rangle, \\ &= (E_a + E_b)\delta_{ac}\delta_{bd} + H_{ab,cd}^{22}, \\ B_{ab,cd} &\equiv (-)\left\langle \Phi \left[a_b a_a,\ \mathcal{H} a_d a_c - a_d a_c \mathcal{H}\right] \Phi \right\rangle \\ &= 4! \cdot H_{abcd}^{40}, \end{aligned} \tag{48}$$

as Eq. (8.200) in Ref. [3]. With these A and B matrices, H_2 can be represented as

$$\begin{aligned} H_2 = \frac{1}{8}\sum_{k\neq l}\sum_{m\neq n} &\Big(Z_{kl}(-)B_{kl,mn}^* Z_{mn} + Z_{kl} A_{kl,mn}^* (-) Z_{mn}^* \\ &+(-)Z_{kl}^* A_{kl,mn} Z_{mn} + Z_{kl}^*(-)B_{kl,mn} Z_{mn}^* \Big). \end{aligned} \tag{49}$$

Thus, finally

$$\begin{aligned} \langle \Phi' \mid \mathcal{H} \mid \Phi' \rangle &\cong H_\Phi - \frac{i}{2}\sum_{k\neq l} \left(H_{kl}^{20*},\ H_{kl}^{20}\right) \begin{pmatrix} Z_{kl} \\ -Z_{kl}^* \end{pmatrix} \\ &+\frac{1}{8}\sum_{a\neq b,\ c\neq d} \left(-Z_{ab}^*,\ Z_{ab}\right) \begin{pmatrix} A_{ab,cd} & -B_{ab,cd} \\ -B_{ab,cd}^* & A_{ab,cd}^* \end{pmatrix} \begin{pmatrix} Z_{cd} \\ -Z_{cd}^* \end{pmatrix} \\ &+\mathcal{O}\left(Z^3\right) \end{aligned} \tag{50}$$

Therefore, the variational principle leads us to conclude that

$$\begin{aligned} \left.\frac{\partial \langle \Phi' \mid \mathcal{H} \mid \Phi' \rangle}{\partial (-) Z_{kl}^*}\right|_{Z=0} &= -iH_{kl}^{20} = 0, \\ \left.\frac{\partial \langle \Phi' \mid \mathcal{H} \mid \Phi' \rangle}{\partial Z_{kl}}\right|_{Z^*=0} &= -iH_{kl}^{20*} = 0. \end{aligned} \tag{51}$$

This condition determines the Bogoliubov transformation: $\hat{\mathcal{W}}^\dagger$ should make both H^{20} and H^{20*} to be zero. In addition, we have still one degree of freedom, the unitary transformation among quasi particles, $a_k' = \sum_l Y_{kl} a_l$, which does not affect the last variational condition. This Y_{kl} can be fixed to diagonalize the last matrix H^{11}.

Summarizing the above discussions, from the variational principle with respect to Eq. (41), Bogoliubov

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[4] This discussion is copied from Sec. 7.3 in Ref. [3], but with some corrections.

[5] If $\mathcal{G}$ was not Hermite, the norm of $|\Phi'\rangle$ cannot conserve. This condition is equivalent to that the operator $i\mathcal{G}$ should be anti-Hermite.

[6] These matrices A and B are indeed QRPA matrices as written in section 8.9 in the textbook [3] by P. Ring and P. Schuck.

transformation $\hat{\mathcal{W}}^\dagger$ must be determined so as to realize

$$\mathsf{H}' \equiv \begin{pmatrix} H^{11} & H^{20} \\ -H^{20*} & -H^{11*} \end{pmatrix} = \hat{\mathcal{W}}^\dagger \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \hat{\mathcal{W}} = \begin{pmatrix} \mathrm{Diag}(E_\mu) & \emptyset \\ \emptyset & -\mathrm{Diag}(E^*_\mu) \end{pmatrix}. \quad (52)$$

where the eigenvalues of H^{11} should be real because of the Hermiticy of h: $E^*_\mu = E_\mu$. With this solution, the total Hamiltonian takes the form,

$$\mathcal{H} = H_\Phi + \frac{1}{2} \left(a^\dagger_\rightarrow,\ a_\rightarrow \right) \mathsf{H}' \begin{pmatrix} a_\downarrow \\ a^\dagger_\downarrow \end{pmatrix} + \mathcal{H}_R = H_\Phi + \sum_\mu E_\mu a^\dagger_\mu a_\mu + \mathcal{H}_R. \quad (53)$$

For actual solution of the Bogoliubov transformation, one needs to solve the diagonalization problem of H:

$$\sum_l \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}_{kl} \begin{pmatrix} U_{lm} \\ V_{lm} \end{pmatrix} = \delta_{km} E_m \begin{pmatrix} U_{km} \\ V_{km} \end{pmatrix}. \quad (54)$$

The above form is usually called as HFB equation. Thus, the HFB energies are obtained as the eigenvalues of H from this equation.

A. Time-dependent version of HFB

The HFB formalism can be naturally extended to the time-dependent (TD) case. First remember that the time-dependent Schrödinger equation, $i\hbar |\Psi(t)\rangle = \mathcal{H} |\Psi(t)\rangle$, is equivalent to the time-dependent variational principle:

$$\delta \left\langle \Psi(t) \left[i\hbar \frac{\partial}{\partial t} - \hat{\mathcal{H}} \right] \Psi(t) \right\rangle = 0. \quad (55)$$

Instead of a general trial state $|\Psi(t)\rangle$, in TD-HFB framework, we consider the TD-Slater quasi-particle (QP) determinant: $|\Psi(t)\rangle \Longrightarrow |\Phi'(t)\rangle$. This $|\Phi'(t)\rangle$ is the vacuum of the TD-quasi particle operators.

In general, $c^\dagger_\mu$ and c_ν can be used as the STATIC basis to represent the TD energy functional. That is,

$$\hat{\mathcal{H}}'(t) = \frac{1}{2} \left[c^\dagger_\rightarrow,\ c_\rightarrow \right] \mathsf{H}(t) \begin{bmatrix} c_\downarrow \\ c^\dagger_\downarrow \end{bmatrix} + \hat{\mathcal{N}}_\Phi [...] + const., = H_\Phi(t) + \frac{1}{2} \left[a^\dagger_\rightarrow(t),\ a_\rightarrow(t) \right] \mathsf{H}'(t) \begin{bmatrix} a_\downarrow(t) \\ a^\dagger_\downarrow(t) \end{bmatrix} + \mathcal{H}_R(t), \quad (56)$$

where $H_\Phi(t) \equiv \langle \Phi'(t) \,|\, \mathcal{H}(t) \,|\, \Phi'(t)\rangle$. Here the supermatrices read

$$\mathsf{H}(t) \equiv \begin{pmatrix} h(t) & \Delta(t) \\ -\Delta^*(t) & -h^*(t) \end{pmatrix}, \quad (57)$$

and

$$\mathsf{H}'(t) \equiv \begin{pmatrix} H^{11}(t) & H^{20}(t) \\ -H^{20*}(t) & -H^{11*}(t) \end{pmatrix} = \hat{\mathcal{W}}^\dagger(t) \mathsf{H}(t) \hat{\mathcal{W}}(t). \quad (58)$$

Of course, the TD-Bogoliubov transformation must satisfy that $\hat{\mathcal{W}}(t)\hat{\mathcal{W}}^\dagger(t) = \hat{1}$ at any time.

Le us consider the TD Hamiltonian given as

$$\hat{\mathcal{H}}'(t) = H_\Phi(t) + \sum_{ij} H^{11}_{ij}(t) a^\dagger_j(t) a_i(t) + \frac{1}{2} \sum_{k \neq l} \left[H^{20}_{kl}(t) \left(a_l(t) a_k(t) \right)^\dagger + \text{h.c.} \right] + ... \quad (59)$$

At $t = 0$, of course, $H^{11}_{ij}(0) = E_i \delta_{ij}$ and $H^{20}_{kl}(0) = 0$. For the quasiparticle operator, its time-evolution is described by the Heisenberg equation:

$$i\hbar \frac{\partial}{\partial t} a_k(t) = \left[\hat{\mathcal{H}}'(t), a_k(t) \right]. \quad (60)$$

If there is no perturation, simply $a_k(t) = e^{itE_k/\hbar} a_k$ and $a^\dagger_l(t) = e^{-itE_l/\hbar} a^\dagger_l$. In this case,

$$\hat{\mathcal{H}}'(t) = H_\Phi + \sum_{ij} e^{it(E_i - E_j)/\hbar} H^{11}_{ij}(t) a^\dagger_j a_i + \frac{1}{2} \sum_{k \neq l} \left[e^{-it(E_k + E_l)/\hbar} H^{20}_{kl}(t) \left(a_l a_k \right)^\dagger + \text{h.c.} \right] + ... \quad (61)$$

Otherwise, when it has a deviation as

$$a^\dagger_k(t) = e^{-itE_k/\hbar} \left[a^\dagger_k + \eta d_k(t) \right],\ d_k(t) = \sum_m D_{km}(t) a_m,$$
$$a_k(t) = e^{itE_k/\hbar} \left[a_k + \eta d^\dagger_k(t) \right],\ d^\dagger_k(t) = \sum_m D^*_{km}(t) a^\dagger_m,$$

then ... (I am writing).

IV. QUASI-PARTICLE RANDOM-PHASE APPROXIMATION (QRPA)

For the nuclear excitations, we often adopt the relativistic QRPA procedure developed in Refs. [1, 4]. Namely, after the relativistic H(F)B solution, the quasiparticle nucleon operators are determined as $a_\rho^\dagger$ and a_σ. Using the QRPA ansatz, the excited state $|\omega\rangle$ is formally given as

$$\hat{\mathcal{H}}\,|\omega\rangle = E_\omega\,|\omega\rangle\,, \quad |\omega\rangle = \hat{\mathcal{Z}}^\dagger(\omega)\,|\Phi\rangle\,, \tag{62}$$

where $|\Phi\rangle$ is the relativistic H(F)B ground state (GS) of the A-nucleon system: $\hat{\mathcal{H}}\,|\Phi\rangle = H_\Phi\,|\Phi\rangle$. This formalism can be always validated as,

$$\begin{aligned} &\hat{\mathcal{Z}}^\dagger(\omega) \equiv |\omega\rangle\langle\Phi|\,, \quad \hat{\mathcal{Z}}(\omega) \equiv |\Phi\rangle\langle\omega|\,, \\ \Longleftrightarrow\ &|\omega\rangle = \hat{\mathcal{Z}}^\dagger(\omega)\,|\Phi\rangle\,, \\ &|\Phi\rangle = \hat{\mathcal{Z}}(\omega)\,|\omega\rangle\,, \quad \hat{\mathcal{Z}}(\omega)\,|\Phi\rangle = 0. \end{aligned} \tag{63}$$

Thus, the Eq. (62) is equivalent to that, for the operators $\hat{\mathcal{Z}}^\dagger(\omega)$ and $\hat{\mathcal{Z}}(\omega)$, they follow

$$\left[\hat{\mathcal{H}},\ \hat{\mathcal{Z}}^\dagger(\omega)\right] = \hbar\omega\hat{\mathcal{Z}}^\dagger(\omega), \quad \left[\hat{\mathcal{H}},\ \hat{\mathcal{Z}}(\omega)\right] = -\hbar\omega\hat{\mathcal{Z}}(\omega), \tag{64}$$

where $\hbar\omega \equiv E_\omega - H_\Phi$. Note also that, when one defines an anti-Hermite operator $\hat{\mathcal{W}}(t)$ as

$$\hat{\mathcal{W}}(t) \equiv \hat{\mathcal{Z}}^\dagger(\omega)e^{-i\omega t} - \hat{\mathcal{Z}}(\omega)e^{i\omega t}, \tag{65}$$

then it follows

$$i\hbar\frac{\partial}{\partial t}\hat{\mathcal{W}}(t) = \left[\hat{\mathcal{H}},\ \hat{\mathcal{W}}(t)\right]. \tag{66}$$

Therefore, considering the time-developed state, $|\Phi'(t)\rangle \equiv e^{\hat{\mathcal{W}}(t)}\,|\Phi\rangle$, it satisfies the same Schrödinger equation of the original-HFB GS, $|\Phi\rangle$, via $\hat{\mathcal{H}}$:

$$i\hbar\frac{\partial}{\partial t}\,|\Phi'(t)\rangle = \hat{\mathcal{H}}\,|\Phi'(t)\rangle\,. \tag{67}$$

Note that the anti-Hermiticity of $\hat{\mathcal{W}}(t)$ is needed to conserve the norm of $|\Phi\rangle$ $(t=0)$ and $|\Phi'(t)\rangle$.

The excitation operator $\hat{\mathcal{Z}}^\dagger(\omega)$ with the QRPA ansatz contains the modes up to the 1QP-1QP channel:

$$\hat{\mathcal{Z}}^\dagger(\omega) = \frac{1}{2}\sum_{\rho\neq\sigma}\left\{X_{\rho\sigma}(\omega)\hat{\mathcal{O}}_{\sigma\rho}^{(J,P)\dagger} - Y_{\rho\sigma}^*(\omega)\hat{\mathcal{O}}_{\sigma\rho}^{(J,P)}\right\}, \tag{68}$$

where $\hat{\mathcal{O}}_{\sigma\rho}^{(J,P)} = [a_\sigma \otimes a_\rho]^{(J,P)}$ coupled to the J^P spin and parity. In the following, for simplicity, we omit J^P:

$$\begin{aligned} &\hat{\mathcal{O}}_{\sigma\rho}^{(J,P)} \longrightarrow a_\sigma a_\rho, \\ &\hat{\mathcal{Z}}^\dagger(\omega) = \frac{1}{2}\sum_{\rho\neq\sigma}\left\{X_{\rho\sigma}(\omega)a_\rho^\dagger a_\sigma^\dagger - Y_{\rho\sigma}^*(\omega)a_\sigma a_\rho\right\}. \end{aligned} \tag{69}$$

Notice that, even though $a_\rho\,|\Phi\rangle = 0$, the second term cannot be omitted: this property does not yet guarantee that $Y_{\rho\sigma}^*(\omega) = 0$. By considering the requirement on $\hat{\mathcal{Z}}^\dagger(\omega)$ as in Eq. (72), indeed, $Y_{\rho\sigma}^*(\omega)$ is shown to be possibly finite. On the other hand, terms of $a_\sigma^\dagger a_\rho$ and $a_\sigma a_\rho^\dagger$ can be neglected in $\hat{\mathcal{Z}}^\dagger(\omega)$, as explained in Sec. IV C.

Then, by solving the matrix form of the QRPA equation, excitation amplitudes are obtained:

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} X(\omega) \\ Y^*(\omega) \end{pmatrix} = \hbar\omega\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} X(\omega) \\ Y^*(\omega) \end{pmatrix}, \tag{70}$$

where A and B are the well-known QRPA matrices [1, 3, 4].

A. Derivation of Eq. (70) from Eq. (64)

As shown in Eq. (64), the excitation operator must satisfy that,

$$\left[\hat{\mathcal{H}}, \hat{\mathcal{Z}}^\dagger(\omega)\right] = \hbar\omega\hat{\mathcal{Z}}^\dagger(\omega) + \hat{\mathcal{N}}_\Phi\left[a^{(4)}\right], \tag{71}$$

where $\hat{\mathcal{N}}_\Phi$ indicates the normal ordering with respect to $|\Phi\rangle$. We neglect these quadruple normal-ordered terms:

$$\left[\hat{\mathcal{H}}, \hat{\mathcal{Z}}^\dagger(\omega)\right] \simeq \hbar\omega\hat{\mathcal{Z}}^\dagger(\omega). \tag{72}$$

For the following works, note that

$$\begin{aligned} \left\langle\Phi\left[a_\nu a_\mu,\ (a_\sigma a_\rho)^\dagger\right]\Phi\right\rangle &= \delta_{\mu\rho}\delta_{\nu\sigma} - \delta_{\mu\sigma}\delta_{\nu\rho}, \\ \left\langle\Phi\left[(a_\nu a_\mu)^\dagger,\ a_\sigma a_\rho\right]\Phi\right\rangle &= \delta_{\mu\sigma}\delta_{\nu\rho} - \delta_{\mu\rho}\delta_{\nu\sigma}. \end{aligned} \tag{73}$$

(i) For $X_{\rho\sigma}(\omega)$, from Eq. (72), one can take that

$$\left\langle\Phi\left[a_\nu a_\mu, \left[\hat{\mathcal{H}}, \hat{\mathcal{Z}}^\dagger(\omega)\right]\right]\Phi\right\rangle = \hbar\omega\left\langle\Phi\left[a_\nu a_\mu, \hat{\mathcal{Z}}^\dagger(\omega)\right]\Phi\right\rangle.$$

The right-hand side of this equation indeed reads

$$\begin{aligned} \frac{RHF}{\hbar\omega} &= \left\langle\Phi\left[a_\nu a_\mu, \hat{\mathcal{Z}}^\dagger(\omega)\right]\Phi\right\rangle \\ &= \frac{1}{2}\sum_{\rho\sigma}X_{\rho\sigma}(\omega)\left\langle\Phi\left[a_\nu a_\mu,\ (a_\sigma a_\rho)^\dagger\right]\Phi\right\rangle \\ &= \frac{1}{2}\sum_{\rho\sigma}X_{\rho\sigma}(\omega)\left(\delta_{\mu\rho}\delta_{\nu\sigma} - \delta_{\mu\sigma}\delta_{\nu\rho}\right) \\ &= \frac{1}{2}\left(X_{\mu\nu}(\omega) - X_{\nu\mu}(\omega)\right) = X_{\mu\nu}(\omega). \end{aligned}$$

The left-hand side can be formulated as

$$\begin{aligned} LHS &= \left\langle\Phi\left[a_\nu a_\mu, \left[\hat{\mathcal{H}}, \hat{\mathcal{Z}}^\dagger(\omega)\right]\right]\Phi\right\rangle \\ &= \frac{1}{2}\sum_{\rho\sigma}X_{\rho\sigma}\left\langle\Phi\left[a_\nu a_\mu,\ \hat{\mathcal{H}}a_\rho^\dagger a_\sigma^\dagger - a_\rho^\dagger a_\sigma^\dagger\hat{\mathcal{H}}\right]\Phi\right\rangle \\ &\quad (-)\frac{1}{2}\sum_{\rho\sigma}Y_{\rho\sigma}^*\left\langle\Phi\left[a_\nu a_\mu,\ \hat{\mathcal{H}}a_\sigma a_\rho - a_\sigma a_\rho\hat{\mathcal{H}}\right]\Phi\right\rangle \\ &= \sum_{\rho<\sigma}X_{\rho\sigma}A_{\mu\nu,\rho\sigma} + \sum_{\rho<\sigma}Y_{\rho\sigma}^*B_{\mu\nu,\rho\sigma}, \end{aligned} \tag{74}$$

where the pair-by-pair matrices, A and B, are defined as

$$A_{\mu\nu,\alpha\beta} \equiv \left\langle \Phi \left[a_\nu a_\mu,\ \hat{\mathcal{H}} a^\dagger_\alpha a^\dagger_\beta - a^\dagger_\alpha a^\dagger_\beta \hat{\mathcal{H}} \right] \Phi \right\rangle, \tag{75}$$
$$A^*_{\mu\nu,\alpha\beta} = \left\langle \Phi \left[a_\beta a_\alpha \hat{\mathcal{H}} - \hat{\mathcal{H}} a_\beta a_\alpha,\ (a_\nu a_\mu)^\dagger \right] \Phi \right\rangle,$$
$$B_{\mu\nu,\alpha\beta} \equiv (-) \left\langle \Phi \left[a_\nu a_\mu,\ \hat{\mathcal{H}} a_\beta a_\alpha - a_\beta a_\alpha \hat{\mathcal{H}} \right] \Phi \right\rangle,$$
$$B^*_{\mu\nu,\alpha\beta} = (-) \left\langle \Phi \left[a^\dagger_\alpha a^\dagger_\beta \hat{\mathcal{H}} - \hat{\mathcal{H}} a^\dagger_\alpha a^\dagger_\beta,\ (a_\nu a_\mu)^\dagger \right] \Phi \right\rangle.$$

See also Eq. (47) in Ref. [1]. Therefore, the first equation reads

$$\sum_{\rho<\sigma} X_{\rho\sigma} A_{\mu\nu,\rho\sigma} + \sum_{\rho<\sigma} Y^*_{\rho\sigma} B_{\mu\nu,\rho\sigma} = \hbar\omega X_{\mu\nu}(\omega). \tag{76}$$

(ii) Similarly, for $Y^*_{\rho\sigma}(\omega)$, one can take that

$$\left\langle \Phi \left[\left[\hat{\mathcal{H}}, \hat{\mathcal{Z}}^\dagger(\omega) \right], (a_\nu a_\mu)^\dagger \right] \Phi \right\rangle = \hbar\omega \left\langle \left[\hat{\mathcal{Z}}^\dagger(\omega), (a_\nu a_\mu)^\dagger \right] \right\rangle.$$

Then, the RHS reads

$$\frac{RHS}{\hbar\omega} = \left\langle \left[\hat{\mathcal{Z}}^\dagger(\omega), (a_\nu a_\mu)^\dagger \right] \right\rangle$$
$$= \frac{1}{2} \sum_{\rho\sigma} (-) Y^*_{\rho\sigma}(\omega) \left[a_\sigma a_\rho, (a_\nu a_\mu)^\dagger \right] = (-) Y^*_{\mu\nu}(\omega).$$

The LHS is given as

$$LHS = \left\langle \Phi \left[\left[\hat{\mathcal{H}}, \hat{\mathcal{Z}}^\dagger(\omega) \right], (a_\nu a_\mu)^\dagger \right] \Phi \right\rangle$$
$$= \frac{1}{2} \sum_{\rho\sigma} X_{\rho\sigma}(\omega) \left\langle \Phi \left[\hat{\mathcal{H}} a^\dagger_\rho a^\dagger_\sigma - a^\dagger_\rho a^\dagger_\sigma \hat{\mathcal{H}}, (a_\nu a_\mu)^\dagger \right] \Phi \right\rangle$$
$$(-) \frac{1}{2} \sum_{\rho\sigma} Y^*_{\rho\sigma}(\omega) \left\langle \Phi \left[\hat{\mathcal{H}} a_\sigma a_\rho - a_\sigma a_\rho \hat{\mathcal{H}}, (a_\nu a_\mu)^\dagger \right] \Phi \right\rangle$$
$$= \sum_{\rho<\sigma} X_{\rho\sigma}(\omega) B^*_{\mu\nu,\rho\sigma} + \sum_{\rho<\sigma} Y^*_{\rho\sigma}(\omega) A^*_{\mu\nu,\rho\sigma}. \tag{77}$$

Finally, the second equation reads

$$\sum_{\rho<\sigma} X_{\rho\sigma} B^*_{\mu\nu,\rho\sigma} + \sum_{\rho<\sigma} Y^*_{\rho\sigma} A^*_{\mu\nu,\rho\sigma} = -\hbar\omega Y^*_{\mu\nu}(\omega). \tag{78}$$

Equations (76) and (78) are equivalent to Eq. (70).

B. Notes on QRPA formalism

(i) Because $a_k |\Phi\rangle = 0$, A and B matrices can be simplified as

$$A_{ab,cd} = \left\langle \Phi \mid a_b a_a \left(\mathcal{H} a^\dagger_c a^\dagger_d - a^\dagger_c a^\dagger_d \mathcal{H} \right) \mid \Phi \right\rangle + 0,$$
$$B_{ab,cd} = \langle \Phi \mid a_b a_a a_d a_c \mathcal{H} \mid \Phi \rangle. \tag{79}$$

Also, these QRPA matrices can be represented in terms of the (relativistic) EDF quantities. For the A matrix, the relevant term of $\hat{\mathcal{H}}$ is $\sum_{i\neq j} \sum_{k\neq l} H^{22}_{ij,kl} a^\dagger_i a^\dagger_j a_l a_k / 4$. Thus,

$$A_{ab,cd} \equiv \left\langle \Phi \left[a_b a_a,\ \mathcal{H} a^\dagger_c a^\dagger_d - a^\dagger_c a^\dagger_d \mathcal{H} \right] \Phi \right\rangle,$$
$$= (E_a + E_b)\delta_{ac}\delta_{bd} + H^{22}_{ab,cd},$$
$$= (E_a + E_b)\delta_{ac}\delta_{bd} + \frac{\partial h_{ab}}{\partial \rho_{cd}}, \tag{80}$$

where $h_{\mu\nu} = \frac{\partial \mathcal{E}}{\partial \rho^*_{\mu\nu}}$. Similarly, for the B matrix,

$$B_{ab,cd} \equiv (-) \langle \Phi \left[a_b a_a,\ \mathcal{H} a_d a_c - a_d a_c \mathcal{H} \right] \Phi \rangle$$
$$= \frac{\partial h_{ab}}{\partial \rho^*_{cd}} = 4! \cdot H^{40}_{abcd}. \tag{81}$$

See also Eq. (47) in Ref. [1].

(ii) If the pairing correlation vanishes in the ground state, QRPA becomes a simple RPA. In this case, $|\Phi\rangle = |\mathrm{HF}\rangle$, and thus, with $(m,n) > \epsilon_{\mathrm{F}}$ (particle states) and $(i,j) \leq \epsilon_{\mathrm{F}}$ (hole states),

$$A_{\mu\nu,\alpha\beta} \longrightarrow A_{mi,nj} = (E_m - E_i)\delta_{mn}\delta_{ij} + \frac{\partial h_{mi}}{\partial \rho_{nj}},$$
$$B_{\mu\nu,\alpha\beta} \longrightarrow B_{mi,nj} = \frac{\partial h_{mi}}{\partial \rho^*_{nj}}. \tag{82}$$

Notice the minus sign for the hole-state energies.

C. Why there are no $a^\dagger_* a_*$ neither $a_* a^\dagger_*$ terms?

In the QRPA ansatz, the excitation operator $\hat{\mathcal{Z}}(\omega)$ does not contain the $a^\dagger_* a_*$ neither $a_* a^\dagger_*$ terms. To confirm this neglectability, let us consider the following operator:

$$\hat{\mathcal{Y}}^\dagger(\omega) = \frac{1}{2} \sum_{\rho\neq\sigma} \left[S_{\rho\sigma}(\omega) a^\dagger_\sigma a_\rho - T^*_{\rho\sigma}(\omega) a_\rho a^\dagger_\sigma \right]. \tag{83}$$

The second term, however, is meaningless: it can be renormalized into the first term by using $a_\rho a^\dagger_\sigma = (-) a^\dagger_\sigma a_\rho$. Then, this $\hat{\mathcal{Y}}^\dagger(\omega)$ should satisfy that

$$\left[\hat{\mathcal{H}}, \hat{\mathcal{Y}}^\dagger(\omega) \right] \simeq \hbar\omega \hat{\mathcal{Y}}^\dagger(\omega). \tag{84}$$

For $S_{\rho\sigma}(\omega)$ in the right-hand side, one can find that

$$\left\langle \Phi \left[a_\alpha,\ a^\dagger_\sigma a_\rho \right] a^\dagger_\beta \mid \Phi \right\rangle = \delta_{\alpha\sigma}\delta_{\beta\rho},$$
$$\Longrightarrow \left\langle \Phi \left[a_\alpha,\ \hbar\omega \hat{\mathcal{Y}}^\dagger \right] a^\dagger_\beta \mid \Phi \right\rangle$$
$$= \hbar\omega \frac{1}{2} \sum_{\rho\neq\sigma} \delta_{\alpha\sigma}\delta_{\beta\rho} S_{\rho\sigma}(\omega) = S_{\beta\alpha}(\omega). \tag{85}$$

However, from the LHS of Eq. (84), one should find that

$$\left\langle \Phi \left[a_\alpha, \left[\hat{\mathcal{H}},\ \hat{\mathcal{Y}}^\dagger(\omega) \right] \ \right] a^\dagger_\beta \mid \Phi \right\rangle = 0, \tag{86}$$

because $\hat{\mathcal{H}} = H_\Phi + \sum_\mu E_\mu a^\dagger_\mu a_\mu + \hat{\mathcal{H}}_R$ after the HFB solution, and both three terms yield zero in this braket product. Consequently, $S_{\beta\alpha}(\omega) = 0$.

D. Strength function

In our recent study, the M1 excitation up to the one-body-operator level is considered. Namely, the A-nucleon M1 operator is given as $\hat{\mathcal{Q}}_\nu(\mathrm{M1}) \equiv \sum_{k\in A} \hat{\mathcal{P}}_\nu^{(k)}(\mathrm{M1})$, where $\hat{\mathcal{P}}_{\nu=0,\pm1}^{(k)}$ is the SP-M1 operator of the kth nucleon. Its strength can be obtained as

$$\frac{dB_{\mathrm{M1}}}{dE_\gamma} = \sum_i \delta(E_\gamma - \hbar\omega_i) \sum_\nu \left| \left\langle \omega_i \,\middle|\, \hat{\mathcal{Q}}_\nu(\mathrm{M1}) \,\middle|\, \Phi \right\rangle \right|^2, \quad (87)$$

for all the positive QRPA eigenvalues, $\hbar\omega_i > 0$. Note that, in this work, we neglect the effect of the meson-exchange current as well as the second QRPA [5–10], which needs further multi-body operations but beyond our present technique.

V. TIME-DEPENDENT VARIATIONAL PRINCIPLE FOR QRPA

Theorem: a general time-dependent equation,

$$i\hbar\partial_t \left|\psi(t)\right\rangle = \hat{\mathcal{H}} \left|\psi(t)\right\rangle, \quad (88)$$

is equivalent to the variational equation,

$$\delta \left\langle \psi(t) \left[i\hbar\partial_t - \hat{\mathcal{H}} \right] \psi(t) \right\rangle = 0. \quad (89)$$

This section is devoted to introduce another derivation of the QRPA equation from the time-dependent variational principle. The QRPA scheme is one approximated case of the above, general variational principle: for trial functionals, instead of general ones, we limit up to the single Slater determinant of the quasi-particle (QP) states. There, the trial functionals are allowed to be time-dependent. However, its deviation from the GS ($t = 0$) is limited up to the 1QP-1QP channel.

We consider the excitation from the HFB GS, $|\Phi\rangle$, by the anti-Hermite time-dependent operator $\hat{\mathcal{F}}^\nu(t)$. That is,

$$\hat{\mathcal{H}}'(t) = \hat{\mathcal{H}} + i\hbar \frac{\partial \hat{\mathcal{F}}^\nu(t)}{\partial t}, \text{ with } \left(\hat{\mathcal{F}}^\nu(t) \right)^\dagger = -\hat{\mathcal{F}}^\nu(t). \quad (90)$$

The corresponding time-development is given as

$$\Longrightarrow \left|\Phi'(t)\right\rangle = \exp\left[-\frac{i}{\hbar} \int_0^t ds \hat{\mathcal{H}}'(s) \right] \left|\Phi\right\rangle, \\ = e^{-itH_\Phi/\hbar} \cdot e^{\hat{\mathcal{F}}^\nu(t)} \left|\Phi\right\rangle, \quad (91)$$

where $H_\Phi = \left\langle \Phi \,\middle|\, \hat{\mathcal{H}} \,\middle|\, \Phi \right\rangle$ can be the scalar quantity already. Namely, this time-development is formally driven by the original Hamiltonian plus the external field, $\hat{\mathcal{H}}'(t) = \hat{\mathcal{H}} + \hat{\mathcal{G}}(t)$, with

$$\hat{\mathcal{G}}(t) \equiv i\hbar \frac{\partial \hat{\mathcal{F}}^\nu(t)}{\partial t}. \quad (92)$$

Notice that $\hat{\mathcal{G}}^\dagger(t) = \hat{\mathcal{G}}(t)$. Also, the operator $\hat{\mathcal{F}}^\nu(t)$ is dimension-less, whereas $\hat{\mathcal{G}}(t)$ has the dimension of energy as well as the Hamiltonian.

In the QRPA ansatz, excitations up to the 1QP-1QP type are taken into account[7]:

$$\hat{\mathcal{F}}^\nu(t) = \frac{1}{2} \sum_{k\neq l} \left[F_{kl}^\nu(t) \left(a_l a_k\right)^\dagger - F_{kl}^{\nu*}(t) a_l a_k \right]. \quad (93)$$

Notice that $k \neq l$ for the excitation. In the following, the excitation strength $F_{ab}^\nu(t)$ and $F_{ab}^{\nu*}(t)$ are assumed to be a perturbation against the initial GS. Namely,

[7] See Eq. (8.199) in Ref. [3].

$\eta^2 \equiv \sum_{a<b} |F^{\nu}_{ab}(t)|^2$ is a small, dimension-less parameter, indicating the typical ratio between the excitation and ground-state energies: $1 \gg \eta^2 \cong (E_{\rm exc.} - H_\Phi)/H_\Phi$.

If the state $|\Phi'(t)\rangle$ is truly the excited eigenstate of $\hat{\mathcal{H}}$, the functional variation of $\left\langle \Phi'(t) \left[i\hbar\partial_t - \hat{\mathcal{H}} \right] \Phi'(t) \right\rangle$ must be zero. In the following, we calculate this quantity.

(1) - *exp. value of* $\hat{\mathcal{H}}$: In analogy to Eq. (50), one can compute the expectation value of the original Hamiltonian with respect to the timely-evolved excited state:

$$\left\langle \Phi'(t) \mid \hat{\mathcal{H}} \mid \Phi'(t) \right\rangle = \left\langle \Phi \mid e^{-\hat{\mathcal{F}}(t)} \hat{\mathcal{H}} e^{\hat{\mathcal{F}}(t)} \mid \Phi \right\rangle$$
$$= H_\Phi + \left\langle \Phi \left[\hat{\mathcal{H}}, \hat{\mathcal{F}}^{\nu}(t) \right] \Phi \right\rangle + \frac{1}{2} \langle \Phi \mid \mathcal{X} \mid \Phi \rangle + \mathcal{O}(\hat{\mathcal{F}}^3), \tag{94}$$

where

$$\mathcal{X} = \mathcal{F}\mathcal{F}\mathcal{H} + \mathcal{H}\mathcal{F}\mathcal{F} - 2\mathcal{F}\mathcal{H}\mathcal{F}$$
$$= \left[\left[\hat{\mathcal{H}}, \hat{\mathcal{F}} \right], \hat{\mathcal{F}} \right] = \left[\hat{\mathcal{F}}, \left[\hat{\mathcal{F}}, \hat{\mathcal{H}} \right] \right] = \left[\hat{\mathcal{F}}, -\left[\hat{\mathcal{H}}, \hat{\mathcal{F}} \right] \right] \tag{95}$$

Here it is also worthwhile to remind that, for the external field,

$$\left\langle \Phi'(t) \mid \hat{\mathcal{G}}(t) \mid \Phi'(t) \right\rangle = \left\langle \Phi \mid e^{-\hat{\mathcal{F}}(t)} i\hbar \frac{\partial \hat{\mathcal{F}}(t)}{\partial t} e^{\hat{\mathcal{F}}(t)} \mid \Phi \right\rangle$$
$$= \left\langle \Phi \mid i\hbar \frac{\partial \hat{\mathcal{F}}(t)}{\partial t} \mid \Phi \right\rangle = 0, \tag{96}$$

since $\langle \Phi \mid a_* a_* \mid \Phi \rangle = \left\langle \Phi \middle| a_*^\dagger a_*^\dagger \middle| \Phi \right\rangle = 0$, and thus,

$$\left\langle \Phi'(t) \mid \hat{\mathcal{H}}'(t) \mid \Phi'(t) \right\rangle = \left\langle \Phi'(t) \mid \hat{\mathcal{H}} \mid \Phi'(t) \right\rangle. \tag{97}$$

Therefore, the time-dependent expectation values of the original $\hat{\mathcal{H}}$ via $|\Phi'(t)\rangle$ is always the same to that of the *total*, time-dependent Hamiltonian, $\hat{\mathcal{H}}'(t) = \hat{\mathcal{H}} + \hat{\mathcal{G}}(t)$. Thus, the HFB-excited state, $|\Phi'(t)\rangle$, must be the eigenstate of the original Hamiltonian $\hat{\mathcal{H}}$, as well as the HFB GS.

For the HFB GS $|\Phi\rangle$, the first-order term in Eq. (94) is approximated to vanish: $\left\langle \Phi \left[\hat{\mathcal{H}}, \hat{\mathcal{F}}(t) \right] \Phi \right\rangle \cong 0$. This is equivalent to that, remembering Eq. (53) after the HFB solution, we neglect the term of $\hat{\mathcal{H}}_R$ for this excitation. The second term in Eq. (94), on the other hand, can be represented as a matrix form:

$$\frac{1}{2} \langle \Phi \mid \mathcal{X} \mid \Phi \rangle$$
$$= \frac{1}{8} \sum_{k \neq l} \sum_{m \neq n} \langle \Phi | \Big\{ F_{kl} \left[(a_l a_k)^\dagger, -\left[\mathcal{H}, (a_n a_m)^\dagger \right] \right] F_{mn}$$
$$+ F_{kl} \left[(a_l a_k)^\dagger, [\mathcal{H}, a_n a_m] \right] F^*_{mn}$$
$$+ F^*_{kl} \left[a_l a_k, [\mathcal{H}, (a_n a_m)^\dagger] \right] F_{mn}$$
$$+ F^*_{kl} \left[a_l a_k, -[\mathcal{H}, a_n a_m] \right] F^*_{mn} \Big\} |\Phi\rangle$$
$$= \frac{1}{8} \sum_{a \neq b} \sum_{c \neq d} [F^{\nu *}_{ab}(t),\ F^{\nu}_{ab}(t)] \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}_{ab,cd} \begin{bmatrix} F_{cd}(t) \\ F^*_{cd}(t) \end{bmatrix}, \tag{98}$$

where the QRPA matrices A and B are defined as the same in Eq. (48)[8].

(2) - On the other side, the time-derivation term reads

$$\left\langle \Phi'(t) \mid i\hbar \frac{\partial}{\partial t} \mid \Phi'(t) \right\rangle = \left\langle \Phi'(t) \left[H_\Phi + i\hbar \frac{\partial \hat{\mathcal{F}}^{\nu}}{\partial t} \right] \Phi'(t) \right\rangle$$
$$= H_\Phi + i\hbar \left\langle \Phi \mid e^{-\hat{\mathcal{F}}} \left(\frac{\partial \hat{\mathcal{F}}^{\nu}}{\partial t} \right) e^{\hat{\mathcal{F}}} \mid \Phi \right\rangle, \tag{99}$$

and taking up to the second order of $\hat{\mathcal{F}}^{\nu}(t)$,

$$= H_\Phi + i\hbar \left\langle \Phi \mid \left[\partial_t \hat{\mathcal{F}}^{\nu}, \hat{\mathcal{F}} \right] \mid \Phi \right\rangle + \hat{\mathcal{O}}\left(\hat{\mathcal{F}}^{\nu 3} \right).$$
$$\cong H_\Phi + \frac{1}{4} \sum_{l \neq k} \left\{ F^{\nu *}_{kl}(t) \left(i\hbar \partial_t F^{\nu}_{kl} \right) + F^{\nu}_{kl}(t) \left(-i\hbar \partial_t F^{\nu *}_{kl} \right) \right\}$$
$$= H_\Phi + \frac{1}{4} \sum_{l \neq k} [F^{\nu *}_{kl}(t),\ F^{\nu}_{kl}(t)]\, i\hbar \partial_t \begin{bmatrix} F^{\nu}_{kl}(t) \\ -F^{\nu *}_{kl}(t) \end{bmatrix}. \tag{100}$$

(3) - From Eqs. (98) and (100), one can formulate

$$\left\langle \Phi'(t) \left[i\hbar \frac{\partial}{\partial t} - \hat{\mathcal{H}} \right] \Phi'(t) \right\rangle$$
$$= \frac{1}{4} \sum_{l \neq k} \sum_{c \neq d} [F^{\nu *}_{kl}(t),\ F^{\nu}_{kl}(t)]\, M_{kl,cd} \begin{bmatrix} F^{\nu}_{cd}(t) \\ F^{\nu *}_{cd}(t) \end{bmatrix}, \tag{101}$$

with

$$M_{kl,cd} = \begin{pmatrix} \hat{1} \cdot i\hbar\partial_t - \frac{A}{2}, & -\frac{B}{2} \\ -\frac{B^*}{2}, & -\hat{1} \cdot i\hbar\partial_t - \frac{A^*}{2} \end{pmatrix}_{kl,cd}. \tag{102}$$

Then, considering the TD variational principle,

$$\frac{\delta}{\delta f(t)} \left\langle \Phi'(t) \left[i\hbar \frac{\partial}{\partial t} - \hat{\mathcal{H}} \right] \Phi'(t) \right\rangle = 0, \tag{103}$$

where $f(t) = F^{\nu}_{ab}(t)$ or $F^{\nu *}_{ab}(t)$, the time-development of the excitation operator should satisfy that

$$\begin{pmatrix} \hat{1} & 0 \\ 0 & -\hat{1} \end{pmatrix} i\hbar\partial_t \begin{bmatrix} F_{kl}(t) \\ F^*_{kl}(t) \end{bmatrix} = \begin{pmatrix} A_{kl,ij} & B_{kl,ij} \\ B^*_{kl,ij} & A^*_{kl,ij} \end{pmatrix} \begin{bmatrix} F_{ij}(t) \\ F^*_{ij}(t) \end{bmatrix}. \tag{104}$$

Or equivalently,

$$i\hbar\partial_t \begin{bmatrix} F_{kl}(t) \\ F^*_{kl}(t) \end{bmatrix} = \begin{pmatrix} A_{kl,ij} & B_{kl,ij} \\ -B^*_{kl,ij} & -A^*_{kl,ij} \end{pmatrix} \begin{bmatrix} F_{ij}(t) \\ F^*_{ij}(t) \end{bmatrix}. \tag{105}$$

Up to this point, the form of $F^{\omega}_{kl}(t)$ for the $a_k^\dagger a_l^\dagger$ term has not been limited.

(f) as final step - Now we limit the time-development form of $F^{\nu}_{kl}(t)$ to the oscillator type. That is, with real constants (p_{ab}, q_{ab}),

$$F^{pq}_{ab}(t) = X_{ab}(p) e^{-itp_{ab}} + Y^*_{ab}(q) e^{itq_{ab}}, \tag{106}$$

---

[8] Indeed, the result (98) can be obtained from a simple replacement, $Z_{ab} = -iF_{ab}$ and $-Z^*_{ab} = iF_{ab}$, in Eq. (50).

or equivalently,

$$\begin{bmatrix} F_{kl}(t) \\ F^*_{kl}(t) \end{bmatrix} = \begin{pmatrix} e^{-ip_{ab}t}X_{kl} \\ e^{-iq_{ab}t}Y_{kl} \end{pmatrix} + \begin{pmatrix} e^{iq_{ab}t}Y^*_{kl} \\ e^{ip_{ab}t}X^*_{kl} \end{pmatrix}, \quad (107)$$

$$\Rightarrow i\hbar\partial_t \left[\dots \right] = \begin{pmatrix} \hbar p_{ab}e^{-ip_{ab}t}X_{kl} \\ \hbar q_{ab}e^{-iq_{ab}t}Y_{kl} \end{pmatrix} - \begin{pmatrix} \hbar q_{ab}e^{iq_{ab}t}Y^*_{kl} \\ \hbar p_{ab}e^{ip_{ab}t}X^*_{kl} \end{pmatrix}.$$

(We neglect the subscriptes ab for (p, q) in the following.) By reformulating this RHS, and by applying it to Eq. (105), we show that

$$\begin{aligned} i\hbar\partial_t [\dots] &= \begin{pmatrix} \hbar p\hat{1} & 0 \\ 0 & \hbar q\hat{1} \end{pmatrix}_{ab,kl} \begin{pmatrix} e^{-ipt}X_{kl}(p) \\ e^{-iqt}Y_{kl}(q) \end{pmatrix} \\ &- \begin{pmatrix} \hbar q\hat{1} & 0 \\ 0 & \hbar p\hat{1} \end{pmatrix}_{ab,kl} \begin{pmatrix} e^{iqt}Y^*_{kl}(q) \\ e^{ipt}X^*_{kl}(p) \end{pmatrix} \quad (108) \\ &= \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}_{ab,kl} \begin{pmatrix} X_{kl}(p)e^{-itp} + Y^*_{kl}(q)e^{itq} \\ Y_{kl}(q)e^{-itq} + X^*_{kl}(p)e^{itp} \end{pmatrix}. \end{aligned}$$

Therefore, by comparing the matrix coefficients, it finally leads us to the general matrix form of the QRPA equation. That is,

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}_{ab,kl} \begin{pmatrix} e^{-ipt}X_{kl} \\ e^{-iqt}Y_{kl} \end{pmatrix} = \begin{pmatrix} \hbar p\hat{1} & 0 \\ 0 & \hbar q\hat{1} \end{pmatrix} \begin{pmatrix} \dots \\ \dots \end{pmatrix}. \quad (109)$$

and its complex-conjugate,

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}_{ab,kl} \begin{pmatrix} e^{iqt}Y^*_{kl} \\ e^{ipt}X^*_{kl} \end{pmatrix} = - \begin{pmatrix} \hbar q\hat{1} & 0 \\ 0 & \hbar p\hat{1} \end{pmatrix} \begin{pmatrix} \dots \\ \dots \end{pmatrix}. \quad (110)$$

Note that the equivalency between Eqs. (109) and (110) is coincident to the anti-Hermiticity of the excitation operator $\hat{\mathcal{F}}^\omega$.

The usual QRPA equation is obtained by determining $p = q = \omega$:

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}_{ab,kl} \begin{pmatrix} X_{kl} \\ Y_{kl} \end{pmatrix} = \hbar\omega \begin{pmatrix} X_{ab} \\ Y_{ab} \end{pmatrix}, \quad (111)$$

Another convention is to determine $p = \omega - it(E_a + E_b)/\hbar$ and $q = \omega + it(E_a + E_b)/\hbar$. This means a frequently-used format of $F^\omega_{ab}(t)$ as

$$F^\omega_{ab}(t) = e^{it(E_a+E_b)/\hbar} \left\{ X_{ab}(\omega)e^{-it\omega} + Y^*_{ab}(\omega)e^{it\omega} \right\}, \quad (112)$$

where E_k is the HFB energy.

A. Interpretation of QRPA (2020.02.08)

From the assumption of $F_{ab}(t)$,

$$\begin{aligned} F_{ab}(t) &= X_{ab}(p)e^{-ipt} + Y^*_{ab}(q)e^{iqt} \\ \Longrightarrow \hat{\mathcal{F}}(t) &= \frac{1}{2}\sum_{a\neq b} \left\{ X_{ab}e^{-ipt} + Y^*_{ab}e^{iqt} \right\} (a_a a_b)^\dagger \\ &- \frac{1}{2}\sum_{a\neq b} \left\{ X^*_{ab}e^{ipt} + Y_{ab}e^{-iqt} \right\} (a_a a_b), \quad (113) \end{aligned}$$

where $X(p)$ and $Y(q)$ are obtained from Eqs. (109) and (110). Thus, the corresponding "external field" in addition to the bare Hamiltonian is give as

$$\begin{aligned} \hat{\mathcal{G}}(t) &\equiv i\hbar\partial_t \hat{\mathcal{F}}(t) \\ &= \frac{1}{2}\sum_{k\neq l} \left[\hbar p X_{kl}e^{-ipt} - \hbar q Y^*_{kl}e^{iqt} \right] (a_l a_k)^\dagger + \text{h.c.} \quad (114) \end{aligned}$$

Here we utilized the anti-Hermiticity of $\hat{\mathcal{F}}^\omega(t)$ to save the calculations. By the way, $\hat{\mathcal{G}}(t)$ can be also interpreted as the *induced* Hamiltonian, from the time-evolution of the quasiparticles. Consequently, the QRPA solution can be linked with the perturbation for the TD-QP solution, which invokes the 2QP-0QP and 0QP-2QP components of the TD-HFB energy for $t > 0$.

It is useful to express the induced Hamiltonian in terms of the QRPA matricies and solution. (I) Now we fix $p = \omega - E/\hbar$ and $q = \omega + E/\hbar$. In this case, the $\hat{\mathcal{G}}(t)$ reads the expected, usual form of the Hamiltonian, containing $e^{iEt/\hbar}$ with $E = E_k + E_l$:

$$\begin{aligned} \hat{\mathcal{G}}(t) &= \frac{1}{2}\sum_{k\neq l} \tilde{G}^{20}_{kl}(t)a^\dagger_k a^\dagger_l + \text{h.c.} \quad (115) \\ &= \frac{1}{2}\sum_{k\neq l} e^{iEt/\hbar} \left[G^{(\omega)20}_{kl}e^{-i\omega t} - G^{(\omega)02*}_{kl}e^{i\omega t} \right] a^\dagger_k a^\dagger_l + \text{h.c.}, \end{aligned}$$

where

$$G^{(\omega)20}_{kl} = (\hbar\omega - E)X_{kl}, \quad G^{(\omega)02*}_{kl} = (\hbar\omega + E)Y^*_{kl}. \quad (116)$$

(II) In parallel, if we fix $p = q = \omega$ in Eqs. (109) and (110), the alternative formula is concluded:

$$\hbar\omega X_{kl} = (AX + BY)_{kl}, \quad \hbar\omega Y^*_{kl} = -(AY^* + BX^*)_{kl}. \quad (117)$$

Notice that the QRPA solution, $(X, Y)_{kl}$ for ω, should be common in the cases (I) and (II), as long as the same QRPA matricies are shared. Therefore, by combining the above results,

$$\begin{aligned} G^{(\omega)20}_{kl} &= (A - E\mathbf{1})X_{kl} + BY_{kl}, \quad (118) \\ G^{(\omega)02*}_{kl} &= -BX^*_{kl} - (A - E\mathbf{1})Y^*_{kl}. \quad (119) \end{aligned}$$

This is the induced Hamiltonian written in the format of Eq. (115). Be careful that $\tilde{G}^{20}_{kl}(t)$ does not need to be real (Hermite) anymore.

VI. FINITE AMPLITUDE METHOD

The detailed formulation of FAM-(Q)RPA can be found in Refs. [2, 11, 12]. We briefly follow these works to arrange the formalism necessary in this work. First, we assume an external time-dependent field inducing the polarization in the HFB ground state. That is,

$$\eta\hat{\mathcal{F}}(t) = \eta \int d\omega \left[\hat{F}(\omega)e^{-i\omega t} + \hat{F}^\dagger(\omega)e^{i\omega t}\right], \qquad (120)$$

where η is an infinitesimal real parameter. In this article, $\hat{F}$ is restricted to have the form of the one-body operator. That is,

$$\hat{F}(\omega) = \sum_{kl} f_{kl}^{(\omega)} c_k^\dagger c_l, \qquad (121)$$

where $c_k^\dagger$ and c_l are the original-particle creation and annihilation operators. It is also worthwhile to represent $\hat{F}(\omega)$ in terms of the Bogoliubov transformation. That is,

$$\hat{F}(\omega) = \frac{1}{2}\sum_{\mu\neq\nu}\left[F_{\mu\nu}^{(\omega)20}(a_\nu a_\mu)^\dagger + F_{\mu\nu}^{(\omega)02}a_\nu a_\mu\right] + \sum_{\mu,\nu} F_{\mu\nu}^{(\omega)11} a_\mu^\dagger a_\nu, \qquad (122)$$

where $a_\mu^\dagger$ and a_ν are the quasiparticle creation and annihilation operators, respectively. The expressions of $F_{\mu\nu}^{20}$, $F_{\mu\nu}^{02}$, and $F_{\mu\nu}^{11}$ in terms of the Bogoliubov transformation is summarized in Appendix B. Note also that, in the level of the linear-response approximation with respect to the HFB ground state (GS)[9], the 3rd term with $(a_*^\dagger a_*)$ in Eq. (122) can be neglected, from the similar discussion in Sec. IV C.

The time evolution of quasi particles is described by the time-dependent Heisenberg equation,

$$i\hbar\frac{\partial}{\partial t}a_\mu(t) = \left[\hat{\mathcal{H}}'(t),\ a_\mu(t)\right]. \qquad (123)$$

Since the external field $\eta\hat{\mathcal{F}}(t)$ invokes a density oscillation from the HFB density at $t = 0$, the self-consistent TD-HFB Hamiltonian can also have an induced oscillation. Remember that, with the HFB solution at $t = 0$, the bare Hamiltonian reads

$$\hat{\mathcal{H}} = H_\Phi + \sum_\mu E_\mu a_\mu^\dagger a_\mu + \hat{\mathcal{H}}_R, \qquad (124)$$

with respect to the $|\Phi\rangle$: $\hat{\mathcal{H}}\,|\Phi\rangle = H_\Phi\,|\Phi\rangle$). On the other hand, the TD Hamiltonian is formulated as

$$\hat{\mathcal{H}}'(t) = \hat{\mathcal{H}} + \eta\hat{\mathcal{K}}(t) + \eta\hat{\mathcal{F}}(t), \qquad (125)$$

with the induced field,

$$\eta\hat{\mathcal{K}}(t) = \int d\omega\eta\left[\hat{K}(\omega)e^{-i\omega t} + \hat{K}^\dagger(\omega)e^{i\omega t}\right],$$
$$\hat{K}(\omega) = \frac{1}{2}\sum_{\mu\neq\nu}\left[K_{\mu\nu}^{(\omega)20}(a_\nu a_\mu)^\dagger + K_{\mu\nu}^{(\omega)02}a_\nu a_\mu\right]. \qquad (126)$$

Notice that the $\hat{F}(\omega)$ and $\hat{K}(\omega)$ have the same structure. Therefore, by using $\hat{\mathcal{D}}(t) = \hat{\mathcal{K}}(t) + \hat{\mathcal{F}}(t)$,

$$\begin{aligned}\hat{\mathcal{H}}'(t) &= \hat{\mathcal{H}} + \frac{\eta}{2}\sum_{k\neq l}\left\{\tilde{D}_{kl}^{20}(t)(a_l a_k)^\dagger + \text{h.c.}\right\}, \\ &= H_\Phi + \sum_\mu E_\mu a_\mu^\dagger a_\mu + \hat{\mathcal{H}}_R \\ &+ \frac{\eta}{2}\int d\omega \sum_{\mu\neq\nu}\left\{e^{-i\omega t}D_{\mu\nu}^{(\omega)20} - e^{i\omega t}D_{\mu\nu}^{(\omega)02*}\right\}(a_\nu a_\mu)^\dagger \\ &+ \frac{\eta}{2}\int d\omega \sum_{\mu\neq\nu}\left\{e^{-i\omega t}D_{\mu\nu}^{(\omega)02} - e^{i\omega t}D_{\mu\nu}^{(\omega)20*}\right\}(a_\nu a_\mu),\end{aligned}$$

where $D_{\mu\nu}^{(\omega)20} \equiv K_{\mu\nu}^{(\omega)20} + F_{\mu\nu}^{(\omega)20}$. Here the last term is h.c. of the 4th term, consistently to that $\hat{\mathcal{H}}(t)$ is Hermite. To extract the coefficient of $(a_l a_k)$ or $(a_l a_k)^\dagger$ term, the famous technique can be useful:

$$\begin{aligned}\eta\tilde{D}_{kl}^{20}(t) &= \left\langle\Phi\left[a_l a_k,\ \hat{\mathcal{H}}'(t)\right]\Phi\right\rangle \qquad (127) \\ &= \eta\int d\omega\left\{e^{-i\omega t}D_{kl}^{(\omega)20} - e^{i\omega t}D_{kl}^{(\omega)02*}\right\},\end{aligned}$$

as well as

$$\begin{aligned}\eta\tilde{D}_{kl}^{02}(t) &= \left(\eta\tilde{D}_{kl}^{20}(t)\right)^* = \left\langle\Phi\left[\hat{\mathcal{H}}'(t),\ a_k^\dagger a_l^\dagger\right]\Phi\right\rangle \qquad (128) \\ &= \eta\int d\omega\left\{e^{-i\omega t}D_{kl}^{(\omega)02} - e^{i\omega t}D_{kl}^{(\omega)20*}\right\}.\end{aligned}$$

We assume that the deviation from the static HFB solution is represented as

$$a_\mu(t) = e^{iE_\mu t/\hbar}\left[a_\mu + \eta d_\mu^\dagger(t)\right], \qquad (129)$$

where the deviation part reads

$$\eta d_\mu^\dagger(t) = \eta\int d\omega\sum_\nu\left[X_{\nu\mu}(\omega)e^{-i\omega t} + Y_{\nu\mu}^*(\omega)e^{i\omega t}\right]a_\nu^\dagger. \qquad (130)$$

Thus, at $t > 0$, the HFB GS is NOT the vacuum anymore: $a_\mu(t)\,|\Phi\rangle = 0 + e^{iE_\mu t/\hbar}\eta\,|d_\mu(t)\rangle$.

By solving Eq. (123) up to the first order in η, it yields the so-called FAM equation [2]:

$$\begin{aligned}\left[E_\mu + E_\nu - \hbar\omega\right]X_{\mu\nu}(\omega) &= -D_{\mu\nu}^{(\omega)20}, \\ \left[E_\mu + E_\nu + \hbar\omega\right]Y_{\mu\nu}(\omega) &= -D_{\mu\nu}^{(\omega)02}. \qquad (131)\end{aligned}$$

Or equivalently,

$$\hbar\omega\begin{pmatrix} X \\ -Y\end{pmatrix}_{\mu\nu} - \begin{pmatrix}(E_\mu+E_\nu)X + K^{20} \\ (E_\mu+E_\nu)Y + K^{02}\end{pmatrix}_{\mu\nu} = \begin{pmatrix}F^{20} \\ F^{02}\end{pmatrix}_{\mu\nu}.$$

The quantities needed to obtain the multi-pole strength are the FAM amplitudes, $X_{\nu\mu}(\omega)$ and $Y_{\nu\mu}(\omega)$, at the excitation energy $\hbar\omega$. Now the problem is how to solve $K_{\mu\nu}^{(\omega)20}$ and $K_{\mu\nu}^{(\omega)02}$.

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[9] This approximation is equivalent to neglect $\mathcal{H}_R$ and to assume $H_\Phi \equiv 0$.

A. Time-dependent U and V matrices

In terms of the Bogoliubov transformation from the original-particle representation, the FAM assumption is expressed as

$$a_m(t) = \sum_l \left(U^\dagger_{ml}(t) c_k + V^\dagger_{ml}(t) c^\dagger_l \right) = \sum_l \left(U^*_{lm}(t) c_l + V^*_{lm}(t) c^\dagger_l \right), \tag{132}$$

and

$$a^\dagger_m(t) = \sum_l \left(V^T_{ml}(t) c_l + U^T_{ml}(t) c^\dagger_l \right) = \sum_l \left(V_{lm}(t) c_l + U_{lm}(t) c^\dagger_l \right). \tag{133}$$

For consistency with Eq. (129), it indeed means

$$U_{km}(t) = e^{-iE_m t/\hbar} \left[U_{km} + \eta ... \right], \quad V_{km}(t) = e^{-iE_m t/\hbar} \left[V_{km} + \eta ... \right]. \tag{134}$$

B. FAM-QRPA to the usual QRPA

Let us consider the expectation value of $\hat{\mathcal{H}}'(t)$ at $t > 0$:

$$\left\langle \Phi'(t) \mid \hat{\mathcal{H}}'(t) \mid \Phi'(t) \right\rangle = \left\langle \Phi'(t) \mid \hat{\mathcal{H}}_0 \mid \Phi'(t) \right\rangle + \left\langle \Phi'(t) \mid \eta \hat{\mathcal{D}}(t) \mid \Phi'(t) \right\rangle. \tag{135}$$

where $\hat{\mathcal{D}}(t) \equiv \hat{\mathcal{K}}(t) + \hat{\mathcal{F}}(t)$. Here the TD state reads

$$|\Phi'(t)\rangle = \exp\left[-\frac{i}{\hbar} \int_0^t ds \hat{\mathcal{H}}'(s) \right] |\Phi\rangle \tag{136}$$
$$= e^{-itH_\Phi/\hbar} \cdot \exp\left[-\frac{i}{\hbar} \eta \int_0^t ds \hat{\mathcal{D}}(s) \right] |\Phi\rangle.$$

By comparing the formalism, we can indeed apply the same discussion in Sec. V. Namely, by replacing

$$\hat{\mathcal{F}}(t) \longrightarrow -\eta \frac{i}{\hbar} \int_0^t ds \hat{\mathcal{D}}(s), \quad \hat{\mathcal{G}}(t) \equiv i\hbar \frac{\partial \hat{\mathcal{F}}(t)}{\partial t} = \eta \hat{\mathcal{D}}(t), \tag{137}$$

we can adopt the formalism in Sec. V. It is worthwhile to note that, by using the expressions of $K^{20}_{\mu\nu}$ and $K^{02}_{\mu\nu}$ in terms of $X_{\mu\nu}(\omega)$ and $Y_{\mu\nu}(\omega)$, one can transform Eq. (131) into the matrix form [2, 12]: as given in Eqs. (118) and (119),

$$K^{(\omega)20}_{\mu\nu} = \sum_{\rho\sigma} \left\{ A_{\mu\nu,\rho\sigma} - (E_\mu + E_\nu) \delta_{\mu\rho} \delta_{\nu\sigma} \right\} X_{\rho\sigma}(\omega) + \sum_{\rho\sigma} B_{\mu\nu,\rho\sigma} Y_{\rho\sigma}(\omega), \tag{138}$$

and

$$K^{(\omega)02}_{\mu\nu}(\omega) = \sum_{\rho\sigma} B^*_{\mu\nu,\rho\sigma} X_{\rho\sigma}(\omega) + \sum_{\rho\sigma} \left\{ A^*_{\mu\nu,\rho\sigma} - (E_\mu + E_\nu) \delta_{\mu\rho} \delta_{\nu\sigma} \right\} Y_{\rho\sigma}(\omega), \tag{139}$$

where A and B are the well-known QRPA matrices [3]. Thus, FAM equation (131) can transform into the famous matrix-QRPA equation[10]:

$$\left[\hbar\omega \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} - \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \right] \begin{pmatrix} X(\omega) \\ Y(\omega) \end{pmatrix} = \begin{pmatrix} F^{20} \\ F^{02} \end{pmatrix}, \tag{140}$$

Solving Eq. (140), however, requires us to compute the QRPA matrices which have large dimensions, and to use impractical resources of computations. The essential trick of FAM-QRPA, which enables us to avoid this demanding process, is that we keep Eq. (131), and solve the FAM amplitudes iteratively with respect to the response of the self-consistent Hamiltonian.

C. Numerical method for FAM-QRPA

The response of the self-consistent Hamiltonian, $\delta H^{20}_{\mu\nu}(\omega)$ and $\delta H^{02}_{\mu\nu}(\omega)$, can be expressed in terms of the induced fields [2]:

$$\begin{aligned} \delta H^{20}_{\mu\nu}(\omega) &= U^\dagger \delta h(\omega) V^* - V^\dagger \delta h(\omega)^T U^* \\ &\quad - V^\dagger \overline{\delta\Delta}(\omega)^* V^* + U^\dagger \delta\Delta(\omega) U^*, \\ \delta H^{02}_{\mu\nu}(\omega) &= U^T \delta h(\omega)^T V - V^T \delta h(\omega) U \\ &\quad - V^T \delta\Delta(\omega) V + U^T \overline{\delta\Delta}(\omega)^* U \end{aligned} \tag{141}$$

with the well-known HFB matrices, U and V [3]. In the original paper of FAM-QRPA [2], the induced fields, δh, $\delta\Delta$ and $\overline{\delta\Delta}$, were given by the numerical functional derivatives. In Ref. [14], on the other side, these fields were obtained based on the explicit linearization in order not to mix the densities with different magnetic quantum numbers K. Thanks to this explicit linearization, the infinitesimal parameter η is no longer needed, and the induced fields can be formulated in the similar manner as the HFB fields. That is, $\delta h(\omega) = h'[\rho_f, \kappa_f, \overline{\kappa}_f]$, $\delta\Delta(\omega) = \Delta'[\rho_f, \kappa_f]$ and $\overline{\delta\Delta}(\omega) = \Delta'[\overline{\rho}_f, \overline{\kappa}_f]$, where h' and Δ' are the linearized fields with respect to the perturbed densities. These densities can be expressed as

$$\begin{aligned} \rho_f(\omega) &= +UX(\omega)V^T + V^* Y(\omega)^T U^\dagger, \\ \overline{\rho}_f(\omega) &= +V^* X(\omega)^\dagger U^\dagger + UY(\omega)^* V^T, \\ \kappa_f(\omega) &= -UX(\omega)^T U^T - V^* Y(\omega) V^\dagger, \\ \overline{\kappa}_f(\omega) &= -V^* X(\omega)^* V^\dagger - UY(\omega)^\dagger U^T. \end{aligned} \tag{142}$$

[10] See the section 8.5.1 in the textbook [3].

The procedures that provide h and Δ for the HFB solution can be also utilized for the linearized fields, h' and Δ', with a minor modification. For the iterative solution, the Broyden method is essentially utilized to obtain the convergence [15, 16].

D. Transition strength

Using the FAM-QRPA amplitudes obtained through the iteration, the multi-pole strength distribution is expressed as

$$\frac{dB(\hat{\mathcal{F}};\omega)}{d\omega} \equiv \sum_{i>0} \left| \left\langle i \left| \hat{\mathcal{F}} \right| 0 \right\rangle \right|^2 \delta(\omega - \Omega_i) = -\frac{1}{\pi} \mathrm{Im} S(\hat{\mathcal{F}};\omega), \tag{143}$$

where $i > 0$ denotes the summation over the states with positive QRPA energies $\Omega_i > 0$, and the response function is given by $S(\hat{\mathcal{F}};\omega) = \mathrm{tr}[f\rho_f]$ [2, 14]. In order to prevent the FAM-QRPA strength from diverging at $\omega = \Omega_i$, we employ a small imaginary part in the energy, $\omega \to \omega_\gamma = \omega + i\gamma$, corresponding to a Lorentzian smearing of $\Gamma = 2\gamma$ [2]. The explicit formulation of this smeared strength can be found in Ref. [12]:

$$S(\hat{\mathcal{F}};\omega_\gamma) = -\sum_{i>0} \left\{ \frac{\left| \left\langle i \left| \hat{\mathcal{F}} \right| 0 \right\rangle \right|^2}{\Omega_i - \omega - i\gamma} + \frac{\left| \left\langle 0 \left| \hat{\mathcal{F}} \right| i \right\rangle \right|^2}{\Omega_i + \omega + i\gamma} \right\}. \tag{144}$$

The contour integration technique is worth to be mentioned: one can obtain the discrete QRPA states or multipole sum rules by taking a suited contour integration of $S(\hat{\mathcal{F}};\omega_\gamma)$ on the complex (ω,γ)-plane [12, 17].

Appendix A: Useful formulas

- Field operator: the fermion field $\hat{\psi}(x)$ in the (effective) Lagrangian can be generally represented with the $c_a^\dagger$ and c_a:

$$\hat{\psi}^\dagger(x) = \sum_a \psi_a^*(x) c_a^\dagger,\ \hat{\psi}(x) = \sum_a \psi_a(x) c_a. \tag{A1}$$

- Commutators:

$$\left[a_k^\dagger a_l,\ a_m^\dagger a_n\right] = \delta_{ml} a_k^\dagger a_n - \delta_{nk} a_m^\dagger a_l.$$
$$\left[a_a^\dagger a_b^\dagger,\ a_d a_c\right] = \delta_{da} a_c a_b^\dagger - \delta_{ca} a_d a_b^\dagger + \delta_{cb} a_a^\dagger a_d - \delta_{db} a_a^\dagger a_c. \tag{A2}$$

- Time-dependent expectation value: if the TD state is given as $|\Phi'(t)\rangle = \exp\left[-it\frac{H_\Phi}{\hbar} + i\eta\hat{\mathcal{J}}(t)\right]|\Phi\rangle$, where $\hat{\mathcal{J}}^\dagger(t) = \hat{\mathcal{J}}(t)$, the expectation value of arbitrary operator $\hat{\mathcal{O}}$ is computed as

$$\left\langle \Phi'(t) \mid \hat{\mathcal{O}} \mid \Phi'(t) \right\rangle = \left\langle \Phi \mid e^{-i\eta\hat{\mathcal{J}}(t)} \hat{\mathcal{O}} e^{i\eta\hat{\mathcal{J}}(t)} \mid \Phi \right\rangle, \tag{A3}$$

since H_Φ is scalar. Expanding it up to the second order, one gets

$$\ldots \simeq \left\langle \Phi \mid \left\{ \hat{\mathcal{O}} - i\eta \left[\hat{\mathcal{J}}(t),\ \hat{\mathcal{O}}\right] + \frac{\eta^2}{2}\left[\hat{\mathcal{J}}(t),\ \hat{\mathcal{O}}\hat{\mathcal{J}}(t) - \hat{\mathcal{J}}(t)\hat{\mathcal{O}}\right] \right\} \mid \Phi \right\rangle. \tag{A4}$$

Note that $\hat{\mathcal{J}}(t)$ must be Hermite, otherwise the norm of $|\Phi\rangle$ $(t = 0)$ and $|\Phi'(t)\rangle$ cannot conserve.

Appendix B: External field

In the main text, we consider the external field of the one-body operator form:

$$\hat{\mathcal{F}} = \sum_{kl} f_{kl} c_k^\dagger c_l = \frac{1}{2} \begin{pmatrix} c_\to^\dagger & c_\to \end{pmatrix} \begin{pmatrix} f & 0 \\ 0 & -f^T \end{pmatrix} \begin{pmatrix} c_\downarrow \\ c_\downarrow^\dagger \end{pmatrix}. \tag{B1}$$

In the following, we omit "→" and "↓" for simplicity. From the Bogoliubov transformation, $\hat{\mathcal{W}}\hat{\mathcal{W}}^\dagger = \mathbf{1}$, this can be reformulated as

$$\hat{\mathcal{F}} = \frac{1}{2} \begin{pmatrix} a_\to^\dagger & a_\to \end{pmatrix} \hat{\mathcal{W}}^\dagger \begin{pmatrix} f & 0 \\ 0 & -f^T \end{pmatrix} \hat{\mathcal{W}} \begin{pmatrix} a_\downarrow \\ a_\downarrow^\dagger \end{pmatrix}.$$

Here the matrix calculation reads

$$\hat{\mathcal{W}}^\dagger \begin{pmatrix} f & 0 \\ 0 & -f^T \end{pmatrix} \hat{\mathcal{W}} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} f & 0 \\ 0 & -f^T \end{pmatrix} \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} U^\dagger f U - V^\dagger f^T V & U^\dagger f V^* - V^\dagger f^T U^* \\ V^T f U - U^T f^T V & V^T f V^* - U^T f^T U^* \end{pmatrix} \equiv \begin{pmatrix} F^{11} & F^{20} \\ F^{02} & -(F^{11})^T \end{pmatrix}, \tag{B2}$$

which is consistent to Eq.(122). Notice also that $(F^{20})^T = -F^{20}$ and $(F^{02})^T = -F^{02}$.

Appendix C: Electro-magnetic transitions

Electromagnetic multi pole transition:

$$\hat{\mathcal{Q}} = \hat{\mathcal{Q}}(X\lambda\mu), \tag{C1}$$

where $X = E(M)$ for the electric (magnetic) mode. Those are given as Eqs. (B.23) and (B.24) in textbook [3]. Namely,

$$\hat{\mathcal{Q}}(E\lambda\mu;\boldsymbol{r}) = e_{\text{eff}} r^{\lambda} Y_{\lambda\mu}(\bar{\boldsymbol{r}}),$$
$$\hat{\mathcal{Q}}(M\lambda\mu;\boldsymbol{r}) = \mu_{\text{N}} \left(\vec{\nabla} r^{\lambda} Y_{\lambda\mu}(\bar{\boldsymbol{r}})\right) \cdot \left(\frac{2g_l}{\lambda+1}\hat{\boldsymbol{l}} + g_s \hat{\boldsymbol{s}}\right),$$

where e_{eff}, μ_N (nuclear magneton), g_l, and g_s are the well-known effective parameters. Usually, $e_{\text{eff}} = e$ (0), $g_l = 1$ (0), and $g_s = 5.586$ (-3.826) for the proton (neutron).

Transition probability per time is given as Eq. (B.72) in Ref. [3]:

$$T(X\lambda\mu; I_i \to I_f) = \frac{8\pi(\lambda+1)}{\lambda[(2\lambda+1)!!]^2} \frac{1}{\hbar} \left(\frac{E_{fi}}{\hbar c}\right)^{2\lambda+1} \cdot B(X\lambda\mu; I_i \to I_f) \quad [s^{-1}], \tag{C2}$$

where $E_{fi} = E_f - E_i$ [11]. Here $B(I_i \to I_f)$ is the reduced transition probability, which can be represented as

$$B(X\lambda\mu; I_i \to I_f) = \frac{1}{2I_i+1} \sum_{\mu M_i M_f} \left| \left\langle I_f M_f \middle| \hat{\mathcal{Q}}(X\lambda\mu) \middle| I_i M_i \right\rangle \right|^2. \tag{C3}$$

Note that its unit is commonly $[e^2 \cdot (\text{fm})^{2\lambda}]$. If both the initial and final states are spherical, this can be reduced as

$$B(X\lambda\mu; I_i \to I_f) = \frac{1}{2I_i+1} \left| \left\langle I_f \middle\| \hat{\mathcal{Q}}(X\lambda) \middle\| I_i \right\rangle \right|^2, \tag{C4}$$

by Wigner-Eckart theorem. In order to evaluate $\left\langle I_f \middle\| \hat{\mathcal{Q}}(X\lambda) \middle\| I_i \right\rangle$ and thus $B(I_i \to I_f)$, one should calculate $\left\langle I_f M_f \middle| \hat{\mathcal{Q}}(X\lambda\mu) \middle| I_i M_i \right\rangle$, at least for one time, for the chosen (M_i, μ, M_f).

[11] Within the MKSA system of units, the right-hand side of Eq.(C2) should be multiplied by $\frac{1}{4\pi\epsilon_0}$ for the electric mode, whereas by $\frac{\mu_0}{4\pi} = \frac{1}{4\pi\epsilon_0 c^2}$ for the magnetic mode. Note also that the definition of α and μ_{N} should be different from those in the CGS-Gauss system.

From Weisskopf's estimation [3, 18], for the electric mode,

$$B(E\lambda\mu; I_i \to I_f) \cong \frac{1}{4\pi} \left(\frac{3}{\lambda+3}\right)^2 \left(1.21 A^{1/3}\right)^{2\lambda} \quad \left[e^2 (\text{fm})^{2\lambda}\right], \tag{C5}$$

whereas, for the magnetic mode,

$$B(M\lambda\mu; I_i \to I_f) \cong \frac{10}{\pi} \left(\frac{3}{\lambda+3}\right)^2 \left(1.21 A^{1/3}\right)^{2\lambda-2} \quad [\mu_{\text{N}}^2 (\text{fm})^{2\lambda-2}], \tag{C6}$$

where $\mu_{\text{N}}^2 \cong 1.102 \times 10^{-2}$ $[e^2 \text{fm}^2]$.

Appendix D: Units and Conventions

We employ the CGS-Gauss system of units in this note. Thus, for example,

$$V_{\text{electron}}(r) = \frac{e}{r}, \quad \text{(Coulomb pot. of an electron)}$$
$$\alpha = \frac{e^2}{\hbar c} \cong \frac{1}{137}, \quad \text{(fine structure constant)}$$
$$\mu_{\text{N}} = \frac{e\hbar}{2m_p c}, \quad \text{(nuclear magneton)}$$

where $m_p \cong 938.272$ MeV$/c^2$ (proton mass). It is useful to remember that $\mu_{\text{N}} \cong 0.105$ $[e \cdot \text{fm}]$.

Spin and Pauli's sigma matricies are determined as

$$\hat{s}_x \equiv \frac{\sigma_1}{2}, \quad \hat{s}_y \equiv \frac{\sigma_2}{2}, \quad \hat{s}_z \equiv \frac{\sigma_3}{2},$$

where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

These satisfy

$$\sigma_i \sigma_j = \delta_{ij} + i\epsilon^{ijk}\sigma_k,$$
$$\sigma_i \sigma_j + \sigma_j \sigma_i = 2\delta_{ij},$$
$$\sigma_i \sigma_j - \sigma_j \sigma_i = 2i\epsilon^{ijk}\sigma_k \Longleftrightarrow [\hat{s}_i, \hat{s}_j] = i\epsilon^{ijk}\hat{s}_k. \tag{D1}$$

The following formula is also useful:

$$(\vec{\sigma} \cdot \boldsymbol{A})(\vec{\sigma} \cdot \boldsymbol{B}) = \boldsymbol{A} \cdot \boldsymbol{B} + i\vec{\sigma} \cdot (\boldsymbol{A} \times \boldsymbol{B}). \tag{D2}$$

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