Continuum quasiparticle random phase approximation for astrophysical direct neutron capture reaction of neutron-rich nuclei

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(Dated: November 3, 2014)

Abstract

We formulate a many-body theory to calculate the cross section of direct radiative neutron capture reaction by means of the Hartree-Fock-Bogoliubov mean-field model and the continuum quasiparticle random phase approximation (QRPA). A focus is put on very neutron-rich nuclei and low-energy neutron kinetic energy in the range of $\mathcal{O}(1\,\text{keV})$ - $\mathcal{O}(1\,\text{MeV})$, relevant for the rapid neutron-capture process of nucleosynthesis. We begin with the photo-absorption cross section and the E1 strength function, then, in order to apply the reciprocity theorem, we decompose the cross section into partial cross sections corresponding to different channels of one- and two-neutron emission decays of photo-excited states. Numerical example is shown for the photo-absorption of $^{142}\text{Sn}$ and the neutron capture of $^{141}\text{Sn}$.

PACS numbers: 21.60.Jz 25.20.Dc 25.60.Tv 26.30.Hj
I. INTRODUCTION

The radiative neutron capture, i.e. \((n, \gamma)\) reaction, is one of the fundamental nuclear reactions essential in various nucleosynthesis models. In the rapid neutron-capture process (r-process), relevant to the origin of heavy elements, the reaction takes place in short-lived neutron-rich nuclei, for which direct experimental measurement of the neutron capture cross section is practically impossible. Naturally, an alternative method to measure the inverse reaction, e.g. the Coulomb dissociation, has been considered, but the actual application is quite limited at present even though the experimental possibilities increase with the advances of the RI beam facilities, see for example [1, 2].

The neutron capture reaction is often classified into two different processes depending on the neutron separation energy or the excitation energy after the capture (see, e.g., [3] as a review). One is the compound process in which formation of compound states after absorption of a neutron is assumed, and statistical models are often employed. The compound process has been adopted to describe the slow and rapid neutron-capture processes which take place in stable nuclei or unstable nuclei with large neutron separation energy sufficient to give excitation energy to form the compound states. The main building blocks of the model is the neutron transmission coefficient for the formation of compound states and the gamma-decay strength function for the statistical gamma decay. Recently new modes of dipole excitation such as the pygmy resonance and the soft dipole excitation [4–7] have attracted attentions since influence of the new modes on the r-process nucleosynthesis was pointed out [8]. Motivated with this possibility, microscopic many-body models of electric multipole responses, developed on the basis of the density functional theories, have been applied to the gamma-ray strength function for the compound process calculations [9–14].

The other is the direct radiative capture process in which a electromagnetic transition is assumed to take place from an initial state including the incoming neutron to bound final states without forming compound states. It is estimated that the r-process nucleosynthesis in very neutron-rich nuclei is dominated by the direct process since the formation of the compound states is not likely in neutron-rich nuclei due to small neutron separation energy and small level density at the threshold [3, 15, 16]. Direct neutron capture calculations [15–23] often assumes a simple potential picture in which the initial and final states are described.
as scattering and bound single-particle states. However, one can expect that the new dipole excitation modes may affect the direct neutron capture process likewise in the case of the compound process. To unveil the effect it is necessary to construct a many-body theory of the direct neutron capture reaction in which the correlations in multipole modes of excitation are taken into account. It is the purpose of the present paper to demonstrate that the quasiparticle random phase approximation provides such a framework.

The random phase approximation based on the density functional models has been one of the most powerful theoretical framework to describe electromagnetic responses of nuclei, including new modes in exotic nuclei (see, e.g., [7] as a review, and references therein). The same is for the photo-absorption cross section. Note here that the photo-absorption reaction may have different final reaction channels if nucleons are allowed to be emitted from the photo-excited states. Among them, a reaction followed by one-neutron emission, i.e., \((\gamma,n)\) reaction, is the inverse process of the relevant \((n,\gamma)\) reaction. It is then possible to evaluate the \((n,\gamma)\) cross section using the reciprocity theorem, provided that one can calculate partial cross sections associated with one-neutron emission decays. We note here a method of Zangwill and Soven [24], which is used to describe the partial photo-absorption cross section of atoms [24] and molecules [25] by means of the continuum RPA. In the case of neutron-rich nuclei, however, the pair correlation plays important roles[6, 26–30], and not only one neutron but also two neutrons can be emitted only with small excitation energy. We shall show in the present paper that the partial photo-absorption cross sections corresponding to individual decay channels can be calculated by applying the Zangwill-Soven method to the continuum quasiparticle random phase approximation (cQRPA)[31–33], a version of QRPA, in which the pair correlation is described with the Bogoliubov theory, and the continuum states relevant to the one- and two-neutron emission are described with the proper scattering boundary condition.

We remark that special cares are required to describe capture of a neutron with very low kinetic energy: the energy range relevant to the r-process is \(E_n \sim O(1 \text{ keV}) - O(1 \text{ MeV})\), corresponding to the temperature \(T \sim O(10^7) - O(10^9)\) K of possible r-process environments, and hence we need a fine energy resolution, which is not required in usual RPA or QRPA descriptions of nuclear responses. It should be noted also that the r-process pass may reach to nuclei close to the neutron drip-line having very small one-neutron separation energy \(S_{1n} \sim 1\)
MeV. In such a case we need wave functions of neutrons up to very large distances from the center of the nucleus. Numerical procedures to meet these requirements are also discussed in the present paper.

II. CONTINUUM QUASIPARTICLE RANDOM PHASE APPROXIMATION FOR DIRECT NEUTRON CAPTURE CROSS SECTION

A. Total photo-absorption cross section in QRPA

We shall briefly recapitulate the quasiparticle random phase approximation (QRPA) and its application to a description of the total photo-absorption cross section in order to provide a basis for later discussion.

The photo-absorption reaction is an excitation of a nucleus caused by the electromagnetic transition. Assuming the dominant electric dipole transition (E1 transition) and the second order perturbation with respect to the photo-nuclear interaction, the cross section is given \[34, 35\] as

\[
\sigma(\gamma) = \frac{16\pi^3 e^2 E_\gamma}{3\hbar c} \sum_k |\langle k | D_0 | 0 \rangle|^2 \delta(E_\gamma - \hbar \omega_k) \tag{1}
\]

with the dipole operator \(\hat{D}_0 = \frac{Z}{A} \sum_p r_p Y_{10}(\hat{r}_p) - \frac{N}{A} \sum_n r_n Y_{10}(\hat{r}_n)\). Here \(|0\rangle\) and \(|k\rangle\) are the ground and excited states of the nucleus with the excitation energy \(\hbar \omega_k\). The cross section \(\sigma(\gamma)\) is proportional to the strength function

\[
S(\hbar \omega) = \sum_k |\langle k | \hat{D}_0 | 0 \rangle|^2 \delta(\hbar \omega - \hbar \omega_k) \tag{2}
\]

with \(E_\gamma = \hbar \omega\), multiplied with the factor \(f(E_\gamma) = 16\pi^3 e^2 E_\gamma / 3\hbar c\).

The strength function is formulated by considering linear response of the system under an external one-body field

\[
\hat{V}_{\text{ext}}(t) = \hat{V}_{\text{ext}} e^{-i\omega t} + \hat{V}_{\text{ext}}^\dagger e^{-i\omega t} \tag{3}
\]

with \(\hat{V}_{\text{ext}} = \hat{D}_0\). In QRPA, the response is described on the basis of the time-dependent Hartree-Fock-Bogoliubov (TDHFB) theory (which may be called also the time-dependent Kohn-Sham-Bogoliubov theory), whose basic equation is

\[
i\hbar \frac{\partial}{\partial t} |\Phi(t)\rangle = (\hat{h}[R(t)] + \hat{V}_{\text{ext}}(t)) |\Phi(t)\rangle. \tag{4}
\]
Here $|\Phi(t)\rangle$ is the time-evolving generalized determinant state and $\hat{h}[R(t)] = \hat{T} + \hat{V}_{\text{mf}}[R(t)]$ is the TDHFB(TDKSB) self-consistent Hamiltonian defined by the variation of the energy density functional $E_{\text{tot}}[R] = \langle \Phi|\hat{T}|\Phi\rangle + E_{x}[R]$ with respect to the generalized density matrix matrix $R$. 

In the following we assume that the functional is written in terms of quasi-local one-body densities. The simplest are the one-body density $\rho(r) = \sum_\sigma \langle \Phi|\psi(\sigma)\psi(\sigma)^\dagger|\Phi\rangle$ and the pair-density $\bar{\rho}(r) = \langle \Phi|\psi(r\sigma)\psi(r\sigma)^\dagger|\Phi\rangle$ and its conjugate $\bar{\rho}^*(r)$ while it is not difficult to take into account other quasi-local densities such as the spin, current, kinetic energy and spin-orbit densities, utilized in the Skyrme functional models\cite{30}. In the following, all these quasi-local densities are denoted as

$$\rho_\alpha(r) = \langle \Phi|\hat{\rho}_\alpha(r)|\Phi\rangle$$

with the index $\alpha$ distinguishing the kinds. We also use a collective notation $\{\rho\}$. Here $\hat{\rho}_\alpha(r)$ are corresponding one-body operators. (In the following we assume that the operators satisfy the (anti) hermiticity $\hat{\rho}_\alpha(r)^\dagger = s_\alpha \hat{\rho}_\alpha(r)$ with $s_\alpha = \pm 1$.) The TDHFB mean-field $\hat{V}_{\text{mf}}$ is then expressed as

$$\hat{V}_{\text{mf}}[\{\rho(t)\}] = \sum_\alpha \int dr v_{\alpha}^{\text{mf}}(r,t) \hat{\rho}_\alpha(r),$$

in terms of the functional derivative $v_{\alpha}^{\text{mf}}(r,t) = \partial E_{x}[\{\rho(t)\}]/\partial \rho_\alpha(r)$. We also assume that the external field is expressed as

$$\hat{V}_{\text{ext}} = \sum_\alpha \int dr v_{\alpha}^{\text{ext}}(r) \hat{\rho}_\alpha(r).$$

Considering the time-evolution in the linear response approximation, we describe the fluctuating part $|\delta \Phi(t)\rangle$ of the state vector $|\Phi(t)\rangle$ around the HFB ground state $|\Phi_0\rangle$:

$$(i\hbar \frac{\partial}{\partial t} - \hat{h}_0) |\delta \Phi(t)\rangle = (\hat{V}_{\text{ext}}(t) + \delta \hat{V}_{\text{ind}}(t)) |\Phi_0\rangle,$$

where

$$\delta \hat{V}_{\text{ind}}(t) = \sum_{\alpha\beta} \int dr \kappa_{\alpha\beta}(r) \delta \rho_\beta(r,t) \hat{\rho}_\alpha(r),$$

is fluctuation in the TDHFB mean-field $\hat{V}_{\text{mf}}[\{\rho(t)\}]$, and is often called the induced field. It arises from fluctuation in the densities $\delta \rho_\alpha(r,t) = \langle \Phi_0|\hat{\rho}_\alpha(r)|\delta \Phi(t)\rangle + \langle \delta \Phi(t)|\hat{\rho}_\alpha(r)|\Phi_0\rangle$. 

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\( \kappa_{\alpha\beta}(r) \) is the residual interaction given as the second derivatives of the functional:

\[
\kappa_{\alpha\beta}(r) = \frac{\partial^2 E_x[\{\rho\}]}{\partial \rho_\alpha(r) \partial \rho_\beta(r)}.
\] (10)

Note that the source of \( |\delta \Phi(t)\rangle \) is not only the external field \( \hat{V}_{\text{ext}}(t) \) but also the induced field \( \delta \hat{V}_{\text{ind}}(t) \), as indicated by Eq. (8). Their sum is called the selfconsistent field [24, 25], which is given in the frequency domain as

\[
\hat{V}_{\text{scf}}(\omega) \equiv \hat{V}_{\text{ext}} + \delta \hat{V}_{\text{ind}}(\omega) = \sum_\alpha \int dr v^{\text{scf}}_\alpha(r,\omega) \hat{\rho}_\alpha(r),
\] (11)

\[
v^{\text{scf}}_\alpha(r,\omega) = v^{\text{ext}}_\alpha(r) + \sum_\gamma \kappa_{\alpha\gamma}(r) \delta \rho_\gamma(r,\omega).
\] (12)

The fluctuating densities \( \delta \rho_\alpha(r, t) \) are governed in the frequency domain by the linear response equation:

\[
\delta \rho_\alpha(r, \omega) = \int dr' \sum_\beta R^{\alpha\beta}_0(r, r', \omega) \left( \sum_\gamma \kappa_{\beta\gamma}(r') \delta \rho_\gamma(r', \omega) + v^{\text{ext}}_\beta(r') \right).
\] (13)

Here \( R^{\alpha\beta}_0(r, r', \omega) \) is the unperturbed response function, which is expressed in the spectral representation as

\[
R^{\alpha\beta}_0(r, r', \omega) = \sum_{i<j} \left[ \frac{\langle 0 | \hat{\rho}_\alpha(r) | ij \rangle \langle ij | \hat{\rho}_\beta(r') | 0 \rangle}{\hbar \omega + i \epsilon - E_i - E_j} - \frac{\langle 0 | \hat{\rho}_\beta(r') | ij \rangle \langle ij | \hat{\rho}_\alpha(r) | 0 \rangle}{\hbar \omega + i \epsilon + E_i + E_j} \right].
\] (14)

Here use is made of the quasiparticle states \( i \) and \( j \), which are Fermionic elementary modes of the static HFB Hamiltonian \( \hat{h}_0 = \hat{T} + \hat{V}_{\text{mf}}[\{\rho_0\}] \), defined by [\( \hat{h}_0, a^\dagger_i \] \( = E_i a^\dagger_i \). \( |0\rangle \) denotes the HFB ground state \( |\Phi_0\rangle \), and \( |ij\rangle \equiv a^\dagger_i a^\dagger_j |\Phi_0\rangle \) are two-quasiparticle states.

The strength function is given in terms of the density response as

\[
S(\hbar \omega) = -\frac{1}{\pi} \text{Im} \int dr \sum_\alpha \bar{v}^{\text{ext}}_\alpha(r) \delta \rho_\alpha(r, \omega).
\] (15)

with \( \bar{v}^{\text{ext}}_\alpha(r) = v^{\text{ext}}_\alpha(r)^* s_\alpha \).

**B. Partial cross sections for specific decay channels**

After absorbing a photon, the excited nucleus may decay by emitting one or multiple nucleon(s) if the excitation energy is larger than the threshold energies for the particle emissions.
We shall formulate here a method to evaluate partial cross sections of the photo-absorption reaction defined for specific decay channels. To this end, we extend the method of Zangwill and Soven\cite{24} that is originally formulated for the continuum RPA theory neglecting the pair correlations. We shall show here that the scheme can be generalized to the case of superfluid nuclei by using the Bogoliubov quasiparticles instead of the single-particle states.

The starting point of the method is to note that the strength Eq.(15) is rewritten as

$$ S(\bar{\hbar}\omega) = -\frac{1}{\pi} \text{Im} \int \int d\mathbf{r} d\mathbf{r}' \sum_{\alpha\beta} \bar{v}^{\text{scf}}_{\alpha}(\mathbf{r}, \omega) R^{\alpha\beta}_{0}(\mathbf{r}, \mathbf{r}', \omega) v^{\text{scf}}_{\beta}(\mathbf{r}', \omega) $$

in terms of the selfconsistent field and the unperturbed response function. The derivation is given in Appendix A. Using the spectral representation for $R^{0}(\omega)$, it is further written as

$$ S(\bar{\hbar}\omega) = -\frac{1}{\pi} \text{Im} \sum_{i>j} \left\{ \frac{|\langle ij | \hat{V}_{\text{scf}}(\omega) |0\rangle|^2}{\hbar\omega + i\epsilon - E_i - E_j} - \frac{|\langle 0 | \hat{V}_{\text{scf}}(\omega) |ij\rangle|^2}{\hbar\omega + i\epsilon + E_i + E_j} \right\} $$

$$ = \sum_{i>j} \frac{|\langle ij | \hat{V}_{\text{scf}}(\omega) |0\rangle|^2 \delta_\epsilon(h\omega - E_{ij}) - |\langle 0 | \hat{V}_{\text{scf}}(\omega) |ij\rangle|^2 \delta_\epsilon(h\omega + E_{ij})}{\hbar\omega + i\epsilon + E_i + E_j} $$

(17)

with a Lorentz function

$$ \delta_\epsilon(h\omega = E_{ij}) \equiv \frac{1}{\pi} \frac{\epsilon}{(h\omega + E_{ij})^2 + \epsilon^2}, \quad E_{ij} = E_i + E_j. $$

We here recall (see Eq.(8)) that the time-dependent field causing evolution of the system includes not only the external field $\hat{V}_{\text{ext}}(t) = \hat{V}_{\text{ext}} e^{-i\omega t} + \hat{V}_{\text{ext}}^\dagger e^{i\omega t}$ but also the induced field $\delta\hat{V}_{\text{ind}}(t)$. This points to that $\langle ij | \hat{V}_{\text{scf}}(\omega) |0\rangle$ is the matrix element for transition from the ground state $|0\rangle$ to a two-quasiparticle state $|ij\rangle$. If we take the limit $\epsilon \to 0$ in which $\delta_\epsilon(E)$ converges to the delta function $\delta(E)$, then we may interpret that each term of Eq.(17) is proportional to

$$ w_{ij} = \frac{2\pi}{\hbar} |\langle ij | \hat{V}_{\text{scf}}(\omega) |0\rangle|^2 \delta(h\omega - E_{ij}), $$

(19)

which represents the transition probability per unit time from the the HFB ground state $|0\rangle$ to a two-quasiparticle state $|ij\rangle$. However, we need to pay attentions to spectral properties of the quasiparticle and two-quasiparticle states in order to give precise interpretations to individual terms.

The quasiparticle eigenstates of the HFB Hamiltonian $\hat{h}_0$ are categorized as either discrete bound states or continuum unbound states\cite{26, 27}. The discrete bound states are states
satisfying $E_i < |\lambda|$ with $\lambda$ being the Fermi energy, and they correspond to bound single-particle orbits which are located around the Fermi energy. We label them with $m, n$ etc. in the following. Those with $E_i > |\lambda|$ are all unbound states belonging to a continuum spectrum, and they describe a scattering nucleon. For the continuum quasiparticle states we use labels $p(E_p), q(E_q)$ etc. with explicit quasiparticle energy. Note that a part of single-particle hole orbits is embedded in the continuum spectrum due to the coupling caused by the pair potential. Such hole-like quasiparticle states are resonances in the HFB model.

Two-quasiparticle states $|ij\rangle$ are categorized in three groups. The first is configurations, labeled $|mn\rangle$, in which two quasiparticles are both discrete bound states. The second is configurations $|mp(E_p)\rangle$ in which one quasiparticle is in a bound state $m$ while the other is unbound continuum state $p(E_p)$. They have a threshold energy $S_1 = |\lambda| + \min E_m$, i.e., the one-particle separation energy. The third is the configurations $|p(E_p)q(E_q)\rangle$ with two particles in the continuum, and the corresponding threshold energy is the two-particle separation energy $S_2 = 2|\lambda|$. Note that $S_1 \leq S_2$.

We decompose the strength function according to these categories as

$$ S(h\omega) = S_d(h\omega) + S_{1c}(h\omega) + S_{2c}(h\omega) $$

with

$$ S_d(h\omega) = \sum_{n>m} \sum_n \left[ |\langle nm | \hat{V}_{\text{scf}}(\omega) |0\rangle|^2 \delta_\epsilon(h\omega - E_n - E_m) 
- |\langle 0 | \hat{V}_{\text{scf}}(\omega) |nm\rangle|^2 \delta_\epsilon(h\omega + E_n + E_m) \right], $$

$$ S_{1c}(h\omega) = \sum_n \sum_p \left[ |\langle np(E_p) | \hat{V}_{\text{scf}}(\omega) |0\rangle|^2 \delta_\epsilon(h\omega - E_n - E_p) 
- |\langle 0 | \hat{V}_{\text{scf}}(\omega) |np(E_p)\rangle|^2 \delta_\epsilon(h\omega + E_n + E_p) \right], $$

$$ S_{2c}(h\omega) = \sum_p \sum_{p>q} \left[ |\langle p(E_p)q(E_q) | \hat{V}_{\text{scf}}(\omega) |0\rangle|^2 \delta_\epsilon(h\omega - E_p - E_q) 
- |\langle 0 | \hat{V}_{\text{scf}}(\omega) |p(E_p)q(E_q)\rangle|^2 \delta_\epsilon(h\omega + E_p + E_q) \right]. $$

Here $\sum_p = \sum_{|\lambda|} \int_{|\lambda|} dE_p$ denotes a summation over continuum quasiparticle states. Adopting the partial wave representation, it is the integral over the quasiparticle energy $E_p > |\lambda|$ and a summation $\sum_p'$ with respect to the angular quantum numbers. We shall then examine properties of individual terms for physical energies $E_\gamma = h\omega > 0$. 

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Let us first consider \( S_{1c}(h\omega) \) which collects contributions of two-quasiparticle configurations \( \{|np(E_p)\}\). These configurations consist of one quasiparticle in a scattering state \( p(E_p) \) and the remaining odd-\( A \) nucleus in a one-quasiparticle state \( |n\rangle = a_n^\dagger |0\rangle \). Now consider excitation energy \( h\omega > E_n + |\lambda| \) larger than the threshold of this configuration. Then the integral range of \( \int_{|\lambda|} dE_p \) includes the peak \( E_p = h\omega - E_n \) of the Lorentz function \( \delta_c(h\omega - E_n - E_p) \) and hence \( \delta_c(h\omega - E_n - E_p) \) can be treated as the delta function while \( \delta_c(h\omega + E_n + E_p) \) gives a contribution vanishing in the limit \( \epsilon \to 0 \). Therefore we find that each summand of \( S_{1c}(h\omega) \) in Eq.(22) represents the probability of populating the one-quasiparticle state \( |n\rangle \) and one particle emitted in the continuum scattering state \( p(E_p) \). With multiplication of the kinematical factor \( f(E_\gamma) \), it is equal to the partial photo-absorption cross section

\[
\sigma_{\gamma\to np}(E_\gamma, E_p) = f(E_\gamma)|\langle np(E_p)|\hat{V}_{\text{scf}}(\omega)|0\rangle|^2\delta(E_\gamma - E_n - E_p)
\]

for one-particle emission decay with the configurations mentioned above. Integrating over the energy \( E_p \), this term gives the on-shell cross section

\[
\sigma_{\gamma\to np}(E_\gamma) = f(E_\gamma)|\langle np(E_p)|\hat{V}_{\text{scf}}(\omega)|0\rangle|^2\delta(E_\gamma - E_n - E_p).
\]

These are, in other words, the partial cross sections for one-particle photo-dissociation.

Concerning \( S_{2c}(h\omega) \), each summand of Eq.(23) represents a partial cross section for a decay with emission of two particles in the scattering states \( p(E_p) \) and \( q(E_q) \):

\[
\sigma_{\gamma\to pq}(E_\gamma, E_p, E_q) = f(E_\gamma)|\langle q(E_p)p(E_p)|\hat{V}_{\text{scf}}(\omega)|0\rangle|^2\delta(E_\gamma - E_p - E_q).
\]

It should be noted that \( S_{1c}(h\omega) \) and \( S_{2c}(h\omega) \) have additional contribution in the energy region of discrete spectrum \( 0 < h\omega < S_1 = |\lambda| + \min E_n \) below the threshold \( S_1 \). This is because the selfconsistent field \( \hat{V}_{\text{scf}}(\omega) \) contains poles at the QRPA discrete eigen frequencies \( \omega = \omega_k \) via the density response \( \delta \rho_\alpha(r,\omega) \), and these pole contributions give rise to the delta function peaks \( \propto \delta(h\omega - h\omega_k) \).

The first term \( S_d(h\omega) \) has slightly different structure since the relevant two-quasiparticle configurations \( mn \) have discrete energies \( E_n + E_m \). It might seem that this term exhibits discrete peaks at energies \( h\omega = E_n + E_m \), but this is not the case. As discussed in Appendix B, \( S_d(h\omega) \) for \( h\omega > S_1 \) (above the threshold energy) vanishes in the limit \( \epsilon \to 0 \). For \( h\omega < S_1 \) (below the threshold), \( S_d(h\omega) \) gives rise to discrete peaks \( \propto \delta(h\omega - h\omega_k) \) as \( S_{1c}(h\omega) \) and \( S_{2c}(h\omega) \) do.
Summarizing, Eqs. (16) and (17) of the strength function enables us to decompose the total photo-absorption cross section, Eq.(1), into the partial photo-absorption cross sections associated with one- and two-particle emission decays. Taking the limit \( \epsilon \to 0 \), we have

\[
\sigma_{\gamma}(E_{\gamma}) = f(E_{\gamma})S(E_{\gamma})
\]

\[
= \sum_{k, \hbar \omega_k < E_{th}} \sigma_k \delta(E_{\gamma} - \hbar \omega_k) + \sum_{n} \sum_{p} \sigma_{\gamma \rightarrow np}(E_{\gamma}) + \sum_{p > q} \sigma_{\gamma \rightarrow pq}(E_{\gamma}, E_p, E_q) \tag{27}
\]

where the partial cross sections \( \sigma_{\gamma \rightarrow np} \) and \( \sigma_{\gamma \rightarrow pq} \) for the one- and two-particle emissions are, apart from the kinematical factor \( f(E_{\gamma}) \), the summands of \( S_{1c}(\hbar \omega) \) and \( S_{2c}(\hbar \omega) \) (Eqs.(22) and (23)), respectively, while the photo-absorption cross sections \( \sigma_k \) to populate the bound excited states \( k \) contain contributions from all of \( S_d(\hbar \omega), S_{1c}(\hbar \omega) \) and \( S_{2c}(\hbar \omega) \).

C. Representation using wave functions and Green’s function of quasiparticles

It is useful to write down the above equations in terms of the quantities in the quasiparticle space and its coordinate representation.

A quasiparticle state has a two-component wave function

\[
\phi_i(\mathbf{r} \sigma) \equiv \begin{pmatrix} \varphi_{1,i}(\mathbf{r} \sigma) \\ \varphi_{2,i}(\mathbf{r} \sigma) \end{pmatrix}, \tag{28}
\]

The matrix elements of the one-body operators \( \hat{\rho}_\alpha(\mathbf{r}) \) are given as

\[
\langle ij | \hat{\rho}_\alpha(\mathbf{r}) | 0 \rangle = \sum_\sigma \phi_1^\dagger(\mathbf{r} \sigma) A_\alpha \phi_{j}(\mathbf{r} \sigma), \tag{29}
\]

\[
\langle 0 | \hat{\rho}_\alpha(\mathbf{r}) | ij \rangle = \sum_\sigma \phi_2^\dagger(\mathbf{r} \sigma) A_\alpha \phi_{i}(\mathbf{r} \sigma), \tag{30}
\]

in terms of \( \phi_i(\mathbf{r} \sigma) \) and its conjugate

\[
\overline{\phi}_i(\mathbf{r} \sigma) \equiv \begin{pmatrix} -\varphi_{2,i}^*(\mathbf{r} \sigma) \\ \varphi_{1,i}^*(\mathbf{r} \sigma) \end{pmatrix}, \tag{31}
\]

where \( \phi_i(\mathbf{r} \sigma) \) is the eigen wave function of the \( 2 \times 2 \) HFB Hamiltonian \( \mathcal{H}_0 \) with the quasiparticle eigen energy \( E_i \) while \( \overline{\phi}_i(\mathbf{r} \sigma) \) is the eigen function of the corresponding negative eigen energy \( -E_i \). \( A_\alpha \) is a local operator acting on the quasiparticle wave functions \( \phi_i(\mathbf{r} \sigma) \) and
\( \overline{\phi}_i(\mathbf{r}\sigma) \). (Note that we follow the convention of the quasiparticle wave function introduced in Ref.\,[31] except that \( \overline{\phi}_i(\mathbf{r}\sigma) \) in this paper replaces \( \overline{\phi}_i(\mathbf{r}\sigma) \) used in the preceding papers\,[31–33].)

We shall use also the quasiparticle Green’s function \( G(E) \equiv (E - H_0)^{-1} \) which is expressed in the spectral representation as

\[
G(\mathbf{r}\sigma, \mathbf{r}'\sigma', E) = \sum_n \left( \frac{\phi_n(\mathbf{r}\sigma)\phi_n^\dagger(\mathbf{r}'\sigma')}{E - E_n} + \overline{\phi}_n(\mathbf{r}\sigma)\overline{\phi}_n^\dagger(\mathbf{r}'\sigma') \right) + G_c(\mathbf{r}\sigma, \mathbf{r}'\sigma', E),
\]

\[
G_c(\mathbf{r}\sigma, \mathbf{r}'\sigma', E) = \int \int \left( \frac{\phi_p(\mathbf{r}\sigma)\phi_p^\dagger(\mathbf{r}'\sigma')}{E - E_p} + \overline{\phi}_p(\mathbf{r}\sigma)\overline{\phi}_p^\dagger(\mathbf{r}'\sigma') \right),
\]

(32)

where \( G_c(E) \) is a part arising from the continuum quasiparticle states.

The partial strength function \( S_{1c}(\hbar\omega) \) associated with the one-particle continuum configurations \( |np(E_p)\rangle \) is then written as

\[
S_{1c}(\hbar\omega) = -\frac{1}{\pi} \text{Im} \sum_n \int \int d\mathbf{r}d\mathbf{r}' \sum_{\sigma\sigma'} \left\{ \left( \phi_n^\dagger(\mathbf{r}\sigma)(\mathcal{V}_{\text{scf}}(\mathbf{r}, \omega))^\dagger G_>(\mathbf{r}\sigma\mathbf{r}'\sigma', \hbar\omega + i\epsilon - E_n)\mathcal{V}_{\text{scf}}(\mathbf{r}', \omega)\overline{\phi}_n(\mathbf{r}'\sigma') \right. \\
+ \left. \overline{\phi}_n(\mathbf{r}'\sigma')\mathcal{V}_{\text{scf}}(\mathbf{r}', \omega)G_>(\mathbf{r}'\sigma'\mathbf{r}\sigma, -\hbar\omega - i\epsilon - E_n)\mathcal{V}_{\text{scf}}(\mathbf{r}, \omega)\overline{\phi}_n(\mathbf{r}\sigma) \right\} \\
= -\frac{1}{\pi} \text{Im} \sum_n \left\{ (\phi_n^\dagger)(\mathcal{V}_{\text{scf}}(\omega))^\dagger G_>(\hbar\omega + i\epsilon - E_n)\mathcal{V}_{\text{scf}}(\omega) |\phi_n\rangle \\
+ (\overline{\phi}_n)(\mathcal{V}_{\text{scf}}(\omega)G_>(-\hbar\omega - i\epsilon - E_n)(\mathcal{V}_{\text{scf}}(\omega))^\dagger |\overline{\phi}_n\rangle \right\},
\]

(33)

where

\[
\mathcal{V}_{\text{scf}}(\mathbf{r}, \omega) \equiv \sum_{\alpha} \mathcal{V}_{\text{scf}}(\mathbf{r}, \omega) A_{\alpha}
\]

(35)
is the self-consistent field acting in the quasiparticle space. We have introduced a shorthand bra-ket notation in the last line of Eq.\,(33). \( G_>(E) \) is a part of \( G_c(E) \) associated with the positive energy continuum states:

\[
G_>(\mathbf{r}\sigma, \mathbf{r}'\sigma', E) \equiv \int \frac{\phi_p(\mathbf{r}\sigma)\phi_p^\dagger(\mathbf{r}'\sigma')}{E - E_p}.
\]

(36)

The strength function for the two-particle continuum is expressed as

\[
S_{2c}(\hbar\omega) = -\frac{1}{\pi} \text{Im} \frac{1}{4\pi i} \int_{C'} dE \left\{ \text{Tr}(\mathcal{V}_{\text{scf}}(\omega))^\dagger G_c(E + \hbar\omega + i\epsilon)\mathcal{V}_{\text{scf}}(\omega)G(E) \\
+ \text{Tr}(\mathcal{V}_{\text{scf}}(\omega))^\dagger G(E)\mathcal{V}_{\text{scf}}(\omega)G_c(E - \hbar\omega - i\epsilon) \right\}.
\]

(37)

using the complex energy integration along the contour \( C' \) shown in Fig.1(a).
FIG. 1: The contours $C'$ and $C$ in the complex quasiparticle energy space $E$, adopted for the integrations in Eqs. (37) and (45). The crosses represent the poles at $E = \pm E_i$ corresponding to the bound quasiparticle states. The thick lines are the branch cuts corresponding to the continuum quasiparticle states.

D. Partial cross sections for one-particle decays

Let us concentrate on the partial cross section for one-particle decay channels to give a concrete expression to be used in numerical calculation.

We rewrite Eq.(34) as

$$S_{1c}(\hbar\omega) = -\frac{1}{\pi} \text{Im} \sum_n (\overline{\phi}_n | V_{\text{scf}}(\omega) | \phi_n) \delta_\epsilon(\hbar\omega - E_n + i\epsilon) + \Delta S_{1c}(\hbar\omega)$$  \hspace{1cm} (38)

with

$$\Delta S_{1c}(\hbar\omega) = -\sum_n \sum_p \left| (\overline{\phi}_n | V_{\text{scf}}(\omega) | \phi_p) \right|^2 \delta_\epsilon(\hbar\omega - E_n + E_p)$$

$$-\sum_n \sum_p \left| (\overline{\phi}_p | V_{\text{scf}}(\omega) | \phi_n) \right|^2 \delta_\epsilon(\hbar\omega + E_n + E_p).$$  \hspace{1cm} (39)

We remark that the second term $\Delta S_{1c}(\hbar\omega)$ vanishes if we take the limit $\epsilon \to 0$ and as far as we consider the excitation energies $\hbar\omega > S_1$ above the one-particle separation energy $S_1 = \min E_n + |\lambda|$. This is because $\hbar\omega \mp E_n + E_p > 2|\lambda| - \max E_n > |\lambda|$, and hence $\delta_\epsilon(\hbar\omega \mp E_n + E_p) \propto \epsilon \to 0$.

In the following we assume that the mean fields in the HFB Hamiltonian $H_0$ is spherically symmetric. We use the partial wave expansion: $\phi_{nljm}(r\sigma) = r^{-1} \phi_{nlj}(r) \mathcal{Y}_{ljm}(\sigma)$ for the bound quasiparticle states, and $G(r\sigma, r'\sigma', E) = \sum_{l'j'm'} (rr')^{-1} G_{l'j'}(r, r', E) \mathcal{Y}_{l'j'm'}^l(r\sigma) \mathcal{Y}_{l'j'm'}^{l'}(r'\sigma')$ for the quasiparticle Green’s function,
where \(ljm\) and \(n\) are angular and radial quantum numbers, respectively. Using these quantum numbers, the partial cross section \(\sigma_{\gamma \rightarrow np}(E_{\gamma})\) for one-particle decay is specified by the quantum number \(el'j'\) of the emitted nucleon in the continuum state (with kinetic energy \(e = E - |\lambda|\)) and the quantum number \(nlj\) of a bound one-quasiparticle state of the remaining odd-\(A\) nucleus, as well as the multipolarity \(L\) of the gamma-ray. The one-particle photo-dissociation cross section for this specific channel is given as

\[
\sigma_{\gamma \rightarrow nlj,l'j'}^{L}(E_{\gamma}) = -\frac{f(E_{\gamma}) (l'j' || Y_L || lj)^2}{2L + 1} \cdot \text{Im} \int_{0}^{R_2} dr \int_{0}^{R_2} dr' \phi_{nlj}^{T}(r) (V_{scf,L}(r, \omega))^{\dagger} G_{e,l'j'}(r, r', \hbar \omega - E_{nlj} + i\epsilon) V_{scf,L}(r', \omega) \phi_{nlj}(r') + \Delta \sigma_{\gamma \rightarrow nlj,l'j'}^{L}(E_{\gamma})
\]

(40)

where \(V_{scf,L}(r, \omega)\) is the radial component of the self-consistent field defined by \(V_{scf}(r, \omega) = V_{scf,L}(r, \omega) Y_{LM}(\hat{r})\), and the continuum part of the Green’s function can be calculated as

\[
G_{c,lj}(r, r', E) = G_{lj}(r, r', E) - \sum_{n} \left\{ \frac{\phi_{nlj}(r)\phi_{nlj}^{T}(r')}{E - E_{nlj}} + \frac{\phi_{nlj}(r)\phi_{nlj}^{T}(r')}{E + E_{nlj}} \right\}.
\]

(41)

by subtracting the contribution of the discrete quasiparticle states from the exact HFB Green’s function \(G_{lj}(E)\). The Green’s function \(G_{lj}(E)\) can be constructed exactly in terms of quasiparticle wave functions regular at the origin, and quasiparticle wave function satisfying the boundary condition at infinity\([31, 37]\). In practice we connect the latter to the Hankel functions at a large radius \(R_2\) (see below). [The Coulomb function should be used in the case of proton emission.] Here \(\Delta \sigma_{\gamma \rightarrow nlj,l'j'}^{L}(E_{\gamma})\) corresponds to a summand in \(\Delta S_{1e}\) in Eq.(39). We calculate this unimportant term (vanishing in the limit \(\epsilon \rightarrow 0\)) by replacing the exact continuum states with discretized continuum states obtained with the box boundary condition at \(r = R_2\).

Equation (40) is given a diagrammatic representation as in Fig[2]. Note that the vertex to the photon is not a bare dipole operator \(\hat{V}_{\text{ext}} = D_0\) but the selfconsistent field \(\hat{V}_{\text{scf}}(\omega)\) which includes the polarization effect caused by the correlation in nuclei via the induced field.

E. Direct neutron capture cross section

The inverse process of the photo-absorption reaction leading to a specific decay channel \((nlj)(el'j')\) is the capture of a nucleon with kinetic energy \(e\) in the partial wave \(l'j'\) by the
\[ \sigma \propto \text{Im} \quad V_{\text{scf}}(\omega) \]

\[ \cdots V_{\text{scf}}(\omega) = \cdots V_{\text{ext}} + \cdots + \delta V_{\text{ind}} \]

FIG. 2: A diagrammatic representation of the partial photo-absorption cross section \( \sigma_{\gamma \rightarrow nlj,l'j'}^L(e_\gamma) \), Eq. (40) and the vertex associated with the selfconsistent field \( V_{\text{scf}}(\omega) \).

odd-\( A \) nucleus with the one-quasiparticle configuration \( (nlj) \), followed by the photon emission populating the ground state of the fused even-\( A \) nucleus. Using the reciprocity theorem, one can calculate the cross section of the inverse process with

\[ \sigma_{\text{cap}}(e) = \frac{1}{2j + 1} \frac{E_\gamma^2}{2mc^2}\sigma_{\gamma \rightarrow nlj,l'j'}^L(E_\gamma), \] (42)

where \( e = E_\gamma - E_{nlj} \) is the nucleon kinetic energy and \( m \) is the nucleon mass. This is nothing but the radiative capture cross section for a nucleon in the partial wave \( l'j' \) captured by the odd-\( A \) nucleus with the one-quasiparticle configuration \( nlj \), followed by an E1 transition to the \( 0^+ \) ground state of the even-\( A \) nucleus.

III. NUMERICAL PROCEDURE

In the following we shall demonstrate the present theory with a numerical example. For this purpose, we take neutron-rich tin isotopes with mass number \( A \sim 140 \), in which one-neutron separation energy is \( S_{1n} \sim \) a few MeV, and hence the direct neutron capture is expected to be dominant in the r-process reaction of these isotopes \[14, 15, 21\]. Another reason of the choice is that we can assume the spherical shape because of the proton magicity.
FIG. 3: Calculated one- and two-neutron separation energies $S_{1n}$ and $S_{2n}$ for even-even Sn isotopes, plotted with solid and dotted lines, respectively. The experimental values are shown with squares and crosses for $S_{1n}$ and $S_{2n}$, respectively.

$Z = 50$ as many Hartree-Fock-Bogoliubov calculations predict.

We employ the Skyrme energy density functional model and the effective pairing interaction of the contact type to construct the HFB ground state and the associated selfconsistent mean-field. The adopted Skyrme parameter set is SLy4, and the density-dependent delta interaction of the mixed type

$$v(1, 2) = V_0 \left( 1 - \frac{\rho(r)}{2\rho_0} \right) \delta(r_1 - r_2)$$

($\rho_0 = 0.16 \text{ fm}^{-3}$) is adopted with the quasiparticle energy cut-off $E_{\text{cut}} = 60 \text{ MeV}$ and the orbital angular momentum cut-off $l_{\text{cut}} = 12$. The adopted force strength $V_0 = 292 \text{ MeV fm}^{-3}$ gives average neutron pairing gap $\Delta_n = 1.25 \text{ MeV}$ for stable isotope $^{120}\text{Sn}$ and $\Delta_n = 0.97 \text{ MeV}$ for $^{142}\text{Sn}$. The proton pairing gap is zero. The radial HFB equation is solved in a spherical box $r < R_1$ with mesh interval $\Delta r = 0.2 \text{ fm}$ under the box boundary condition $\phi_{i}|_{r=R_1} = 0$ with the box radius $R_1 = 20 \text{ fm}$, which is sufficiently large for bulk quantities such as the total binding energy to converge. The calculation reproduces rather well the experimental one- and two-neutron separation energies, $S_{1n}$ and $S_{2n}$, of the even-$N$ tin isotopes, as shown in Fig. 3 and it predicts $S_{1n} \approx 2\text{MeV}$ for $A > 140$. 
The continuum QRPA calculation is performed as follows. We adopt the Landau-Migdal approximation in evaluating the linear response: we consider only the fluctuations in the local density and local pair density, and we employ the Landau-Migdal parameters $F_0(r)$ and $G_0(r)$ in the local density approximation for the particle-hole residual interaction. We solve the linear response equation

$$\delta \rho_{\alpha L}(r, \omega) = \int_0^{R_2} dr' \sum_\beta R_{0, L}^{\alpha \beta}(r, r', \omega) \left( \sum_\gamma \kappa_{\beta \gamma}(r') \frac{1}{r^2} \delta \rho_{\gamma L}(r', \omega) + v_{\beta L}^{\text{ext}}(r') \right)$$

in the radial coordinate space. For the unperturbed response function, we use the representation using the quasiparticle Green’s function:

$$R_{0, L}^{\alpha \beta}(r, r', \omega) = \frac{1}{4\pi i} \int_C dE \sum_{l_j, l_j'} \frac{(l_j' y L \parallel l_j)^2}{2L + 1} \left\{ \text{Tr} A_{\alpha} G_{l_j' j}(r, r', E + \hbar \omega + i\epsilon) A_{\beta} G_{l_j j}(r, r, E) \
+ \text{Tr} A_{\alpha} G_{l_j j}(r, r', E) A_{\beta} G_{l_j' j}(r, r, E - \hbar \omega - i\epsilon) \right\}$$

in order to treat the continuum quasiparticle states with the proper boundary condition. The contour $C$ is the one shown in Fig.1(b).

In finding a numerical solution of the linear response equation (44) (using a matrix form with radial mesh points), and also performing numerical integration in Eq.(40), we need a large radial space so that we can evaluate the matrix element $\langle np(E_p) \mid \hat{V}_{\text{scf}}(\omega) \mid 0 \rangle$ accurately for scattering state $p(E_p)$ and weakly bound quasiparticle state $n$. We specify this space with a radius $R_2$. We found that a choice $R_2 = R_1 = 20$ fm provides reasonable results, which however are not sufficiently converged for the photo-absorption cross sections with low-energy neutron emission. However, we cannot simply enlarge the HFB cut-off radius $R_1$ since numerical solution for a quasiparticle state with large quasiparticle energy exhibits an exponential growth of error when the radial HFB equation is integrated toward large $r$ ($\gtrsim 25$ fm in the present case), as discussed by Bennaceur and Dobaczewski. To avoid this problem, we adopt the following two prescriptions. i) For the cut-off radius $R_2$ used in Eqs. (44) and (40), we choose a value larger than $R_1$, while keeping $R_1$ for the HFB calculation. We neglect the HFB mean-fields in calculating wave functions in the interval $R_1 < r < R_2$ since this potential cut-off is known to stabilize significantly the numerical solution of quasiparticle wave functions. The potential cut-off can be justified except for nuclei with very small binding energies $\ll 1$ MeV and with very long tails of the density and the pair density extended to far distances. ii) We introduce a smaller cut-off energy $E_{\text{cut, out}}$
for the upper boundary of the Contour integral in Eq.(45) in evaluating the unperturbed response function \( R_{0,L}^{\alpha\beta}(r,r',\omega) \) at large distances so that the above numerical problem does not come into play. In practice, we use \( E_{\text{cut, out}} = 10 \text{ MeV} \) for \( r' > R_1 \) while the original cut-off value \( E_{\text{cut}} = 60 \text{ MeV} \) is used for \( r' < R_1 \). We found that this choice gives a convergence with respect to \( E_{\text{cut, out}} \). We also found that the convergence of the cross section with respect to \( R_2 \) is obtained with \( R_2 = 30 \text{ fm} \). In evaluating the unperturbed response function, necessary for the QRPA calculation, we use a small but finite value of the imaginary constant \( \epsilon = 0.05 \text{ MeV} \), corresponding to a smearing width of 100 keV in the strength function.

One needs to evaluate the partial photo-absorption cross sections and the neutron capture cross sections with very fine energy resolution if one wants to apply to the astrophysical problems since the relevant energy scale of the neutron kinetic energy is \( \epsilon \sim 1 \times 10^{-3} - 1 \text{ MeV} \). For this purpose, we use a very small imaginary constant \( \epsilon = 1 \times 10^{-8} \text{ MeV} \) for the Green’s function appearing in Eq.(40), thus allowing description of the neutron scattering states with energy resolution \( \sim \epsilon \).

**IV. NUMERICAL EXAMPLE**

Figure 4 shows the calculated E1 strength \( dB(E1)/dE \equiv 3 \sum_k |\langle k| D_0 |0\rangle|^2 \delta(E - \hbar\omega_k) = 3S(E) \) plotted as a function of the excitation energy \( E \). A large fraction of the strength is distributed around \( E \sim 10 - 17 \text{ MeV} \), corresponding to the giant dipole resonance. The strength is also seen between \( E \sim 10 \text{ MeV} \) and the one-neutron separation energy \( S_{1n} \), and it is of our interest in this study. Significant fluctuation or fine structure in the GDR region is seen. They reflect bound proton particle-hole configurations and neutron configurations involving quasiparticle resonances with narrow width. These fine structures might disappear if we take into account the spreading width arising from coupling to more complex configurations, e.g. four quasiparticle configurations etc. If we simulate the spreading width using a finite value of the smearing width, the E1 strength strength distribution becomes smooth as illustrated by the dashed curve, obtained with the smearing width of \( \gamma = 1 \text{ MeV} \).

Figures 5 and 6 show calculated total and partial photo-absorption cross sections. The total photo-absorption cross section \( \sigma_\gamma(E_\gamma) \), the dotted curve in Fig.5 is proportional to \( EdB(E1)/dE|_{E=E_\gamma} \) and hence it has basically the same structure as the E1 strength function.
FIG. 4: Calculated E1 strength function $dB(E1)/dE$ in $^{142}$Sn. The solid curve is the strength obtained with a smearing width $\gamma = 2\epsilon = 100$ keV, while the dashed curve is for a smearing width of 1 MeV. The long and short arrows indicate the one- and two-neutron separation energies $S_{1n}$ and $S_{2n}$, respectively.

Open decay modes of the excited $1^{-}$ states are one- and two-neutron emissions. The one- two-neutron separation energies are low: $S_{1n} = E_{3p_{3/2}} + |\lambda_n| = 2.246$ MeV and $S_{2n} = 2|\lambda_n| = 2.796$ MeV, respectively ($E_{3p_{3/2}}$ is the quasiparticle energy of the neutron $3p_{3/2}$ state). The one-proton separation energy $S_{1p} = |e_{1p_{1/2}}| = 18.191$ MeV is located at much higher energy. The partial photo-absorption cross section for one-neutron emission decay is shown with the solid curve in Fig[5] It is seen that the partial cross section for two-neutron decay becomes a sizable fraction for $E_{\gamma} \gtrsim 3.5$ MeV. The fraction of one-neutron cross section becomes significantly small as the energy increases although the one-neutron decay survives at energies where the two-neutron decay channels are open. We remark also that the one-neutron partial cross section exhibits non-trivial energy dependence which arises from the configuration mixing in the dipole states. For instance, the fine structures seen around $E_{\gamma} \sim 9 - 17$ MeV can be explained only with mixing among proton particle-hole and neutron two-quasiparticle configurations.

The one-neutron decay is further decomposed into individual decay channels specified with different neutron configurations. In the present case bound neutron quasiparticle states are
3\textit{p}_{3/2} and 3\textit{p}_{1/2} states with quasiparticle energies \( E_{3\textit{p}_{3/2}} = 0.848 \text{ MeV} \) and \( E_{3\textit{p}_{1/2}} = 1.257 \text{ MeV} \) while all the other quasiparticle states are in the continuum \( E > |\lambda_n| \). Therefore configurations corresponding to the final states of one-neutron decay are the \( 3\textit{p}_{3/2} \) state coupled with continuum \( s_{1/2}, d_{5/2} \) and \( d_{3/2} \) states, combined in total spin and parity \( 1^- \) (abbreviated as \( 3\textit{p}_{3/2} \otimes cs_{1/2}, 3\textit{p}_{3/2} \otimes cd_{3/2} \) and \( 3\textit{p}_{3/2} \otimes cd_{5/2} \), hereafter), and similarly, \( 3\textit{p}_{1/2} \otimes cs_{1/2} \) and \( 3\textit{p}_{1/2} \otimes cd_{3/2}, \) involving the \( 3\textit{p}_{1/2} \) state. The first three are decay channels in which the one-quasiparticle state \( 3\textit{p}_{3/2} \), the calculated ground state of \( ^{141}\text{Sn} \), is populated while the last two are those populating the one-quasiparticle state \( 3\textit{p}_{1/2} \), the only bound excited state in \( ^{141}\text{Sn} \) obtained in the present HFB calculation. The partial photo-absorption cross sections for these decay channels are plotted in Fig.6. The decay channels with population of the ground \( 3\textit{p}_{3/2} \) state open at \( E_\gamma = E_{3\textit{p}_{3/2}} + |\lambda_n| = S_{1n} \) while the channels populating the \( 3\textit{p}_{1/2} \) state open at \( E_\gamma = E_{3\textit{p}_{1/2}} + |\lambda_n| = 2.655 \text{ MeV} \), higher than \( S_{1n} \) by 409 keV. It is seen that the probability of populating the excited \( 3\textit{p}_{1/2} \) state is finite but much smaller than that populating the ground state \( 3\textit{p}_{3/2} \). We show in Fig.7 the decay branching ratio. It is seen that the branching ratio varies with excitation energy, displaying monotonic increase (decrease) of the two-neutron (one-neutron) decay branches.

Focusing on the ground state decays (the solid curves in Fig.6), we find an apparent
feature that the channel with the escaping neutron in the $s_{1/2}$ wave dominates over those in the $d$ waves at the lowest energies close to the threshold. At higher energies $E_\gamma > \sim \, 3$ MeV, the channel with the $d$-wave neutron dominates.

It is interesting to compare this result with a simple model corresponding to single-particle transitions in the Hartree-Fock approximation. For the latter, we perform a calculation neglecting the pairing correlation and the RPA correlation caused by the residual interactions. In practice we perform the HFB calculation using a reduced paring interaction strength $V_0 = 120$ MeV fm$^{-3}$, which leads to a very small average neutron pairing gap $\Delta_n = 0.048$ MeV, and calculate the partial photo-absorption cross sections using Eq. 40 in which the selfconsistent field $V_{\text{scf}}(\omega)$ is replaced with the bare dipole operator. The result is shown in Fig. 8 for the decay channels populating the $3p_{3/2}$ and $3p_{1/2}$ state of the daughter $^{141}\text{Sn}$. (The cross section for the $3p_{1/2}$ state is calculated to be practically zero.)

Several clear differences are seen between Figs. 6 and 8. First, the one-neutron separation energy is higher in the full calculation by about 1.5 MeV than that in the Hartree-Fock single-particle model. This due to the pair correlation which has an effect to give the even-$N$...
nucleus $^{142}$Sn more binding energy. The separation energy in the Hartree-Fock approximation is essentially the single-particle energy -0.883 MeV of the $3p_{3/2}$ orbit while the pair correlation increases the separation energy via the quasiparticle energy $E_{3p_{3/2}}$ and the Fermi energy $\lambda_n$. Second, the probability to populate the $3p_{1/2}$ state is finite in the full HFB + QRPA calculation while it is zero in the Hartree-Fock approximation. This is because the single-particle $3p_{1/2}$ orbit is partially occupied in the HFB description of the pair correlated ground state of $^{142}$Sn while the occupation is zero in the unpaired Hartree-Fock approximation. Third, the cross sections have non-trivial energy dependence in the full calculation while the energy-dependence in the Hartree-Fock single-particle transitions are quite simple. The non-trivial energy dependence is due to the RPA correlation and the configuration mixing as we already mentioned above. The simple structure in the single-particle transitions, on the other hand, can be understood even in an analytical way [47, 48].

Finally we show in Fig.9 direct neutron capture cross section for $^{141}$Sn in the ground state having the one-quasiparticle configuration $3p_{3/2}$ and with the $E1$ decay populating the $0^+$ ground state of $^{142}$Sn. It is calculated for neutron kinetic energies from $e = 1$ keV to 8 MeV using Eq.(42) and the partial photo-absorption cross sections shown in Fig.6. We see that
FIG. 8: Partial photo-absorption cross sections for specific channels of one-neutron emission decay, obtained by neglecting the pairing and RPA correlations. Decays populating the $3p_{3/2}$ and $3p_{1/2}$ states of the daughter $^{141}$Sn are evaluated, but the cross sections for the $3p_{1/2}$ state is calculated to be zero in this null pairing case.

The $s$-wave capture is dominant at low energies $E \lesssim 1$ MeV as expected. It is also seen that the energy dependence at very low energies $E \lesssim 100$ keV obeys the power-low scaling $\sigma \propto E^{l-1/2}$ (with $l$ being the orbital angular momentum of the partial wave). This threshold behavior arises from the low-energy asymptotics of the neutron continuum quasiparticle states in the $s_{1/2}$, $d_{3/2}$ and $s_{3/2}$ waves. Note, however, that their absolute magnitudes as well as behaviors at higher energies differ from the simple single-particle model, as we discussed above. The threshold scaling behavior would have been affected if the $s$- and $d$-wave neutron had low-energy resonance or virtual state in $E \lesssim 100$ keV, or if the QRPA correlation would have exhibited narrow resonances in this energy region. Such situation is not seen in the present example.

V. CONCLUSIONS

The quasiparticle random phase approximation (QRPA) combined with the Hartree-Fock-Bogoliubov mean-field model or the nuclear density functional theory is one of the most powerful frameworks to describe the electro-magnetic responses and the photo-absorption reaction of neutron-rich nuclei. In this paper, we have extended this framework to describe the direct radiative neutron-capture reaction of neutron-rich nuclei, one of key reactions in the
FIG. 9: Neutron capture cross sections for three different entrance channels, consisting of the ground state with the $3p_{3/2}$ configuration of $^{141}\text{Sn}$ and an incident neutron in the partial waves $s_{1/2}$, $d_{3/2}$ and $d_{5/2}$, populating $1^-$ states decaying to the ground state of $^{142}\text{Sn}$. The horizontal axis is the neutron kinetic energy $e$. 

We have formulated a method to calculate partial photo-absorption cross sections corresponding to individual channels of one- and two-nucleon emission decays. It is a generalization of the method of Zangwill and Soven, originally formulated in the continuum RPA for unpaired systems, to the case of the continuum QRPA suitable for pair correlated nuclei. We select one-neutron emission channels in which the decay populates the daughter nucleus in its ground state. We then use the reciprocity theorem to transform the partial photo-absorption cross section to the radiative neutron capture cross section. With improved numerical procedure, we made it possible to evaluate the neutron capture cross section at very low neutron kinetic energies of $O(1 \text{ keV})$ and for nuclei with small neutron separation energies. The theory also enables us to evaluate the branching ratio of the one- and two-neutron emission decays of the photo-excited states.

Performing numerical calculations for the photo-absorption of $^{142}\text{Sn}$ and the neutron-
capture of $^{141}$Sn, we have shown that the pairing and the RPA correlations influence the results significantly. It is shown also that the threshold behavior of the cross sections, governed by the partial waves of the emitted/incoming neutron, emerges in the present theory.

We remark that in the present work we have neglected the gamma decays from excited to excited states. For example, we find a low-lying collective $2^+_1$ state below the neutron separation energy in the present QRPA calculation, but possible E1 transition from the $1^-$ state populated by the neutron capture to the collective $2^+_1$ state is not described in the present formalism. It is a future problem to extend the formalism to include this kind of transitions. We also note that neutron capture of even-$N$ isotopes needs to be described in a separate way.

Acknowledgment

The author thanks T. Nakatsukasa, K. Ogata and K. Yabana for useful discussion. This work is supported by Grant-in-Aid for Scientific Research from Japan Society for Promotion of Science No. 23540294 and No. 26400268.

Appendix A

We shall show a derivation of Eq. (16).

We note first

$$S(\hbar \omega) = -\frac{1}{\pi} \text{Im} \int dr \sum_{\alpha} \bar{v}_{\alpha}^{\text{ext}}(r, \omega) \delta \rho_\alpha(r, \omega)$$

$$= -\frac{1}{\pi} \text{Im} \int dr \sum_{\alpha} \left( \bar{v}_{\alpha}^{\text{scf}}(r, \omega) - \sum_\gamma \bar{\kappa}_{\alpha\gamma}(r) \delta \rho_\gamma(r, \omega) \right) \delta \rho_\alpha(r, \omega)$$

$$= -\frac{1}{\pi} \text{Im} \int dr \sum_{\alpha} \bar{v}_{\alpha}^{\text{scf}}(r, \omega) \delta \rho_\alpha(r, \omega)$$

$$+ \frac{1}{\pi} \frac{1}{2i} \left[ \int dr \sum_{\alpha, \gamma} \bar{\kappa}_{\alpha\gamma}(r) \delta \rho_\gamma(r, \omega) \right] \delta \rho_\alpha(r, \omega)$$

$$\quad - \int dr \sum_{\alpha, \gamma} \bar{\kappa}_{\alpha\gamma}^*(r) \delta \rho_\gamma(r, \omega) \delta \rho_\alpha(r, \omega) \right] , \quad (46)
where
\[ \bar{\kappa}_{\alpha\gamma}(r) \equiv (\kappa_{\alpha\gamma}(r))^* s_\alpha = \frac{\partial^2 E}{\partial \rho_\alpha^*(r) \partial \rho_\beta(r)} s_\alpha = \frac{\partial^2 E}{\partial \rho_\alpha(r) \partial \rho_\beta^*(r)}. \] (47)

Using the symmetry
\[ \bar{\kappa}_{\alpha\beta}(r)^* = \bar{\kappa}_{\beta\alpha}(r), \] (48)
we find that the term in the parenthesis in the last expression in Eq.(46) vanishes. We note also that the linear response equation (13) is written as
\[ \delta \rho_\alpha(r, \omega) = \int dr' \sum_\beta R_{\alpha\beta}^{0}(r, r', \omega) v_{\beta}^{\text{scf}}(r, \omega). \] (49)

Inserting this into Eq.(46), we obtain Eq.(16).

**Appendix B**

In this appendix, we discuss spectral property of \( S_d(h\omega) \) in Eq.(21):
\[ S_d(h\omega) = \frac{1}{\pi} \text{Im} \sum_{n > m} \left\{ \frac{\langle nm | V_{\text{scf}}(\omega) | 0 \rangle^2}{h\omega - E_n - E_m + i\epsilon} - \frac{\langle 0 | V_{\text{scf}}(\omega) | nm \rangle^2}{h\omega + E_n + E_m + i\epsilon} \right\}. \] (50)

It is tempting to expect delta function peaks at \( h\omega = \pm(E_n + E_m) \), the energies of the two-quasiparticle states consisting of bound quasiparticle states \( m \) and \( n \), but this is not the case.

To show this, we return to the linear fluctuation in the state vector \( |\delta \Phi(\omega)\rangle = e^{-i\omega t} |\Phi(\omega)\rangle + e^{i\omega t} |\Phi(-\omega)\rangle \) obeying Eq.(8), which reads in the frequency domain
\[ \left( h\omega - \hat{h}_0 + i\epsilon \right) |\delta \Phi(\omega + i\epsilon')\rangle = V_{\text{scf}}(\omega + i\epsilon') |\Phi_0\rangle. \] (51)
The strength function \( S_d(h\omega) \) is then written as
\[ S_d(h\omega) = \sum_{n > m} \frac{\epsilon}{\pi} |\langle nm | \delta \Phi(\omega + i\epsilon')\rangle|^2 - \frac{\epsilon}{\pi} |\langle \delta \Phi(-\omega - i\epsilon')|nm\rangle|^2. \] (52)

We remark here that all the quantities related to the linear response, e.g., \( |\delta \Phi(\omega)\rangle \) and \( \delta \rho_\alpha(\omega) \) inherit the spectral property of the linear response equation (13), which exhibits the QRPA eigen modes. Therefore, in the discrete energy region \( h\omega < S_1 \), the matrix elements
\langle nm|\delta \Phi(\omega)\rangle \text{ and } \langle \delta \Phi(-\omega)|nm \rangle \text{ have poles } \propto 1/(\hbar \omega \mp \hbar \omega_k + i\epsilon), \text{ and hence } S_d(\hbar \omega) \text{ displays delta function peaks at the discrete QRPA eigen energies } \pm \hbar \omega_k \text{ in the limit } \epsilon \to 0:

\begin{equation}
S_d(\hbar \omega) = \sum_{k, \hbar \omega_k < S_1} s_k^d \delta(\hbar \omega - \hbar \omega_k) - s_k^d \delta(\hbar \omega + \hbar \omega_k).
\end{equation}

On the other hand, in the continuum energy region \( \hbar \omega > S_1 \), the matrix elements \( \langle nm|\delta \Phi(\omega + i\epsilon')\rangle \) and \( \langle \delta \Phi(-\omega - i\epsilon)|nm \rangle \) are continuous functions of real \( \omega \). Therefore \( S_d(\hbar \omega) \) is proportional to \( \epsilon \) for sufficiently small \( \epsilon \), and it vanishes in the limit \( \epsilon \to 0 \) and for \( \hbar \omega > S_1 \).

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