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Continuum dipole response near the threshold and the direct neutron capture cross section at astrophysical energies

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Abstract. We apply the continuum quasiparticle random phase approximation to calculate the direct neutron capture cross section relevant to the r-process nucleo-synthesis. The electric dipole strength function in an even-even n-rich nucleus is decomposed with respect to the channels of direct neutron decays. Using the detailed balance relation, the partial dipole strengths are converted to obtain the direct neutron-capture cross sections. Numerical examples are given for 142 Sn.

1. Introduction

The rapid neutron capture process is physics that plays a central role in understanding the origin of heavy elements in our universe[1,2]. The r-process passes through neutron-rich nuclei in essentially all the mass regions of the nuclear chart via various reactions and decays, such as the neutron capture, the photo-absorption, the beta-decay and the fission. Besides experimental efforts to produce and measure the relevant neutron-rich nuclei in the advanced RI beam facilities, a large number of theoretical studies have been performed aiming at quantitative description of the relevant nuclear structures and reactions. The nuclear density functional theories are, in our opinion, one of the most promising nuclear models for this purpose since they provide not only accurate description of the nuclear masses but also the nuclear responses for the weak and electromagnetic interactions. In the present work, I show that the nuclear density functional theory also has a ability to describe the key nuclear reaction in the r-process, i.e., the direct neutron capture.

The low-energy neutron capture reaction may be modeled using two different mechanisms[2]. One is the statistical mechanism: it is assumed that the capture of a neutron leads to formation of compounds states which then decay by statistical E1-gamma transitions. The Hauser-Feshbach statistical reaction theory is usually adopted, and the gamma-ray strength function associated with the compounds states is one of the key quantity. Recently microscopic calculations of the strengh functions based on the quasiparticle random phase approximation to the density functional theories or their extensions [3,4] are applied in order to improve predictabilities. The other is the direct neutron capture mechanism where the gamma-decay occurs immediately after the neutron capture. The relative importance of the two mechanisms depends on the neutron separation energy $S_n[2,5]$. For nuclei near the stability line, relevant to the s-process, the separation energy $S_n \sim 8$ MeV is so large that the Bohr's compounds states are formed because

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI. Published under licence by IOP Publishing Ltd 1 of the high level density. In this situation the statistical mechanism dominates. The neutron-rich nuclei involved in the r-process, however, have much smaller separation energy $S_n \sim O(1)$ MeV, and it is suggested that the direct neutron capture dominates[5]. The neutron single-particle model is often adopted in calculating the direct neutron capture cross section[6-8]. However, the neutron-rich nuclei is known to exhibit anomalous features in the electromagnetic responses, for instance, the enhanced E1 response arising from the pygmy dipole resonance. The enhanced E1 response and the pygmy resonance may imply correlation or collectivity of a new kind although their properties are under current investigates. We need to go beyond the single-particle model in order to include these effects. It is the purpose of our study to provide such a description on the basis of the recent advances in the nuclear density functional theories.

2. The continuum QRPA and the E1 strength function

The starting point of our formulation is the continuum quasiparticle random phase approximation (QRPA) [9] applied to the Skyrme-Hartree-Fock-Bogoliubov model. It is a linear response theory describing excitations of a nucleus caused by a perturbing external field V_{ext} , the electric dipole field in our case. Adopting the time-dependent Hartree-Fock-Bogoliubov theory as a fundamental framework to describe the time-evolution of the system, the perturbation causes fluctuations in the particle density and the pair density, which in turn induce fluctuations in the selfconsistent Hartree-Fock-Bogoliubov mean fields. The selfconsistent relation between these quantities is written as

$$\begin{pmatrix} \delta\rho(r,\omega)\\ \delta\tilde{\rho}(r,\omega)\\ \delta\tilde{\rho}^{*}(r,\omega) \end{pmatrix} = \int dr' \left(R_{0}^{\alpha\beta}(r,r',\omega) \right) \begin{pmatrix} \delta\Gamma(r',\omega) + v_{ext}(r')\\ \delta\tilde{\Delta}(r',\omega)\\ \delta\tilde{\Delta}^{*}(r',\omega) \end{pmatrix}$$
(1)

where $\delta\rho(r,\omega)$ and $\delta\tilde{\rho}(r,\omega)$ are the fluctuations in the density and the pair density, respectively, and $\delta\Gamma(r,\omega) = (\partial^2 E_{edf}/\partial^2 \rho) \,\delta\rho(r,\omega)$ and $\delta\tilde{\Delta}(r,\omega) = (\partial^2 E_{edf}/\partial^2 \tilde{\rho}) \,\delta\tilde{\rho}(r,\omega)$ are the induced Hartree-Fock and pair fields derived from the energy density functional E_{edf} . Propagations of the quasiparticles excited by the external field and the induced selfconsistent fields bring about the fluctuation in the densities. This is described by the response function $R_0^{\alpha\beta}(r,r',\omega)$, which is expressed in terms of the quasiparticle Green's function G(r,r',E). It is then straightforward to obtain the strength function for the E1 operator: we solve Eq.(1) for the dipole field $v_{ext}(r) = (Z/A\delta_{\tau p} - N/A\delta_{\tau n})r$, and then evaluate the E1 strength function

$$S_{E1}(\omega) = \sum_{k} |\langle 1^{-}k | v_{ext} | 0^{+} \text{gs} \rangle|^{2} \delta(\Omega_{k} - \omega) = -\frac{1}{\pi} \text{Im} \int dr v_{ext}(r) \delta\rho(r, \omega)$$
(2)

where $|k\rangle$ is the QRPA excited states with excitation energy Ω_k . The quantum numbers are omitted in the above equations. The details of the continuum QRPA are given in Refs.[9-11], and in the present work we follow Ref.[10]. The photo-absorption cross section via the E1 gamma's is given by

$$\sigma_{\gamma}(E_{\gamma}) = \frac{16\pi^3 e^2}{9\hbar c} E_{\gamma} S_{E1}(E_{\gamma}). \tag{3}$$

3. The direct neutron capture cross section

Let us outline how we use the continuum QRPA to calculate the direct neutron capture cross section. It is noted here that the excited states populated by the photo-absorption have a decay branch of direct one-neutron emission if the excitation energy exceeds the neutron separation energy. The continuum QRPA has an advantage, compared to the standard QRPA frameworks, that it enables to describe the direct neutron decays. This is because the neutron wave functions

in the continuum energy region (i.e. the quasineutron states above the separation threshold) are connected to the scattering waves in the external region. We wish to decompose the total photoabsorption cross section into partial cross sections corresponding to different decay channels. Once this is achieved, we can convert the partial photo-absorption cross sections to the direct neutron capture cross sections by using the detailed balance relation since the direct neutron capture with the E1 gamma decay is the inverse process of the E1 photo-absorption followed by one-neutron emission.

We apply and extend the prescription of Zangwill and Soven [12,13] for this decomposition. In the preceding works, the method is formulated in the framework of the continuum RPA which have been applied to the photo-absorption and associated electron emission of molecules and atomic clusters [12,13]. In the present case, however, the nucleus is in the superfluid phase caused by the neutron pair correlation. A clear difference is that once the pairing is switched on both one and two neutron emissions are allowed. Concerning the one-neutron decays, the channels are specified by the partial wave of the emitted neutron (i.e. the quasineutron states in the continuum) and the states of the residual A - 1 nucleus, which correspond to the bound one-quasineutron states.

The partial E1 strength function specific to a one-neutron decay channel with the residual quasiparticle configuration i is calculated as

$$S_{E1,1c,i}(\omega) = -\frac{1}{\pi} \operatorname{Im} \int \int dr dr' \bar{\phi}_{\tilde{i}}(r)^{\dagger} (\mathcal{V}_{scf}(r,\omega))^{\dagger} G_{>}(r,r',\omega-i0-E_i) \mathcal{V}_{scf}(r',\omega) \bar{\phi}_{\tilde{i}}(r') + (\operatorname{backward})$$
(4)

where $\phi_i(r)$ is the two-component wave function of the bound quasiparticle state *i* with energy E_i , and $\bar{\phi}_{\bar{i}}(r)$ being its negative energy counter part. $\mathcal{V}_{scf}(r,\omega)$ is the 2×2 matrix representation of the selfconsistent fields $(\delta\Gamma(r,\omega) + v_{ext}(r'), \delta\tilde{\Delta}(r,\omega), \delta\tilde{\Delta}^*(r,\omega))$. $G_>(r,r',E)$ is the quasiparticle Green's function which describe propagation of the quasiparticle with continuum spectrum, i.e., the neutron escaping from the nucleus under the influence of the Hartree-Fock-Bogoliubov mean-fields. One can show that the partial strength $S_{E1,1c,i}(\omega)$ is equivalent to

$$S_{E1,1c,i}(\omega) = \sum_{p \in \text{cont.}} |\langle ip | \mathcal{V}_{scf}(\omega) | 0 \rangle|^2 \delta(E_i + E_p - \omega)$$
(5)

where $|\langle ip|\mathcal{V}_{scf}(\omega)|0\rangle|^2$ is the partial E1 strength in which the final state is the one-quasineutron state *i* (the residual A-1 nucleus) plus the continuum neutron state *p*. The crucial point is that the operator $\mathcal{V}_{scf}(\omega)$ appearing in these expressions includes, in addition to the bare E1 operator $v_{ext}(r)$, the induced fields $\delta\Gamma(r,\omega)$ and $\delta\tilde{\Delta}(r,\omega)$ representing effects of the RPA correlations or the collectivity of the excited states at energy $E_x = \omega$.

4. Results

We have performed numerical calculations for a very neutron-rich tin isotope 142 Sn. This is an isotope whose one-neutron separation energy is calculated to be around 2 MeV, and it may be located around the r-process path. We adopt the parameter set SLy4 for the Skyrme functional and the density-dependent delta interaction model of the mix type for the effective pairing interaction. We use the spherical HFB + continuum QRPA code[10] adopting the mesh representation in the radial coordinate, and the space size is chosen as $R_{max} = 20$ fm. The Landau-Migdal approximation is introduced for the residual interaction to obtain the induced Hartree-Fock field in the continuum QRPA calculation. The solid curve in Fig.1 is the total E1 strength function obtained with Eqs.(1) and (2). Here the strength function is smoothed with the smearing width of 1 MeV.

The large strengths distributed around $E_x \sim 10 - 18$ MeV correspond to the giant dipole resonance. In addition, a significant amount of strength is seen at low excitation energies



Figure 1. The E1 strength function of 142 Sn as a function of the excitation energy, calculated with the Skyrme-HFB plus continuum QRPA method (the solid curve). The dotted curve is the partial E1 strength function for the decay channels with direct one-neutron emission. The smoothing width is chosen to 1 MeV. The arrows indicate the one- and two-neutron separation energies.

 $E_x \sim 2-8$ MeV located just above the one-neutron separation energy $S_{1n} = 2.25$ MeV. Our model predicts that the low-lying E1 strength appears in neutron-rich isotopes heavier than 132 Sn, and the strength increases with the neutron excess, suggesting larger photo-absorption cross section and larger direct neutron capture cross section.

There are only two bound quasineutron states in the present HFB calculation. They correspond to the $3p_{3/2}$ and $3p_{1/2}$ orbits located above the N = 82 shell gap. Correspondingly the A-1 system ¹⁴¹Sn, described as one-quasineutron states in the present model, has only two bound states $3/2^-$ and $1/2^-$ having the $3p_{3/2}$ and $3p_{1/2}$ quasineutron configurations, respectively. The 1^- excited states of ¹⁴²Sn populated by the E1 gamma can decay via one-neutron emission leaving the $3p_{3/2}$ or $3p_{1/2}$ quasineutron state of ¹⁴¹Sn. The dotted curve in Fig.1 is the partial E1 strength, Eq.(4), associated with these decay channels. It is noted here that the partial strength with one-neutron decay is only a small fraction of the total E1 strength at excitation energies $E_x \gtrsim 5$ MeV. We found that the direct two-neutron decay, i.e. the decay mode emitting two-neutrons and populating directly the ground state of the A-2 system ¹⁴⁰Sn dominates among the remaining E1 strength. This channel has a considerable fraction since the calculated two-neutron separation energy is small $S_{2n} = 2.80$ MeV, and the presence of the pair correlation makes many of the hole-like quasiparticle states unbound.

Let us now focus on the strength near the neutron separation energy $E_x \sim S_{1n}$. Figure 2 shows the partial E1 strengths for the direct one-neutron decay channels. Here the total strength is decomposed according to both the partial waves of the escaping neutron $(s_{1/2}, d_{3/2} \text{ or } d_{5/2})$ and the configurations $(3p_{1/2} \text{ or } 3p_{3/2})$ of the populated state of the residual ¹⁴¹Sn. Here we adopt a negligibly small smoothing width 10^{-6} MeV in order to guarantee a sufficiently fine



Figure 2. The partial E1 strength functions in ¹⁴²Sn for different channels of the direct oneneutron decay. The solid curves are for the decays populating the $3p_{3/2}$ one-quasineutron state in ¹⁴¹Sn with one neutron emission in the partial waves $s_{1/2}$, $d_{3/2}$, and $d_{5/2}$. The dotted curves are for the decays to the $3p_{1/2}$ one-quasineutron state in ¹⁴¹Sn and the neutron partial waves $s_{1/2}$ and $d_{3/2}$. The smoothing width is 10^{-6} fm.

energy resolution. At energies just above the one-neutron separation energy, only the channels populating the $3p_{3/2}$ configuration are open since the $3p_{3/2}$ configuration has lower energy than $3p_{1/2}$ (i.e. it is the ground state of ¹⁴¹Sn). It is seen in Fig.2 that the partial strengths for decays with the *s*-wave neutron steeply rise at the threshold energy. This is consistent with the energy dependence $\propto (E - E_{th})^{l+1}$ which is expected from the low-energy behavior of the scattering neutron waves[6-8].

Using the partial E1 strength functions thus obtained and Eq.(3), we calculate the partial photo-absorption cross sections $\sigma(\gamma + A \rightarrow (A - 1)_i + n_p)$. We then relate this to the direct neutron capture cross section $\sigma((A - 1)_i + n_p \rightarrow \gamma + A)$ using the detailed balance:

$$\sigma((A-1)_i + n_p \to \gamma + A) = S_{J_A J_{A-1}} \frac{k_\gamma^2}{k_n^2} \sigma(\gamma + A \to (A-1)_i + n_p) \tag{6}$$

with k_{γ} and k_n being the photon and neutron momenta, and $S_{J_A J_{A-1}}$ is a spin factor. Provided that the ground state of ¹⁴¹Sn is the one-quasineutron state $3p_{3/2}$, the direct neutron capture of ¹⁴¹Sn followed by the E1 transition to the ground state of ¹⁴²Sn takes place for neutron partial waves $s_{1/2}$, $d_{3/2}$ and $d_{5/2}$. The calculated direct neutron capture cross sections are plotted in Fig.3 for an interval of neutron kinetic energy from $E_n = 0.01$ MeV (10 keV) to 6 MeV, which is relevant to the r-process nucleo-synthesis. Note that the typical temperature of the astronomical environment is order of $T \sim 10^9$ K, corresponding to $E_n \sim k_B T \sim 0.1$ MeV.

It is seen that the s-wave capture is dominant, and the d-wave capture cross section decreases as the energy becomes low. The energy dependence is consistent with $\propto E_n^{l-1/2}$ (the dashed



Figure 3. The calculated direct neutron capture cross sections of ¹⁴¹Sn, plotted as a function of the captured neutron energy E_n . Plotted is the cross section divided by the spin factor $S_{J_A J_{A-1}}$ in Eq.(6).

lines), which comes from the low-energy behavior of the partial E1 strength $S_{E1} \propto E_n^{l+1/2}$ seen in Fig. 3. We found that the calculated cross sections are influenced by the RPA correlations. Such effects are taken into account via the induced fields $\delta\Gamma$ and $\delta\Delta$ in the selfconsistent field \mathcal{V}_{scf} used in Eqs.(4) and (5). Consequently the calculated cross sections differ from the values evaluated in the simple single-particle models.

In conclusion, the density functional theory plus the continuum QRPA provides a new scheme to calculate the direct neutron capture cross section relevant to the r-process nucleo-synthesis.

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