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Neutron Transfer Reactions for Deformed Nuclei Using Sturmian Basis States

V.G. Gueorguiev[1,2], **J.E. Escher**[3]
[1]Ronin Institute, NJ, USA
[2]Institute for Advanced Physical Studies, Sofia, Bulgaria
[3]Lawrence Livermore National Laboratory, Livermore, California, USA

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Abstract. We study the spin-parity distribution P(J^π,E) of ^{156}Gd excited states above the neutron separation energy $S_n = 8.536$ MeV [1] that are expected to be populated via the 1-step neutron pickup reaction ^{157}Gd(^{3}He,^{4}He)^{156}Gd. In analogy with the rotor plus particle model [2], we view excited states in ^{156}Gd as rotational excitations built on intrinsic states consisting of a neutron hole in the ^{157}Gd core; that is, a neutron removal from a deformed Woods-Saxon type single-particle state [3] in ^{157}Gd. The particle-core interaction usually dominated by a Coriolis coupling are accounted via first order perturbation theory [4]. The reaction cross section to each excited state in ^{156}Gd is calculated as coherent contribution using a standard reaction code [5] based on spherical basis states. The spectroscopic factor associated with each state is the expansion coefficient of the deformed neutron state in a spherical Sturmian basis along with the spherical form factors [4]. The total cross section, as a function of the excitation energy, is generated using Lorentzian smearing distribution function. Our calculations show that, within the assumptions and computational modeling, the reaction ^{3}He+^{157}Gd $\rightarrow$ ^{4}He+^{156}Gd* has a smooth formation probability P(J^π,E) within the energy range relevant to the desired reaction ^{155}Gd+n $\rightarrow$ ^{156}Gd*. The formation probability P(J^π,E) resembles a Gaussian distribution with centroids and widths that differ for positive and negative parity states.

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1 Introduction and Motivation

Understanding the production of the heavy elements is one of the most important challenges for nuclear astrophysics [6]. Multiple nucleosynthesis processes play a role and unravelling their respective contributions to the observed abundances of the elements requires knowledge of the neutron-induced reactions on unstable nuclei. Unfortunately, measuring these cross sections in a laboratory environment is a very difficult, if not impossible, task because of the technical and practical problems associated with the use of an unstable nuclei. There have

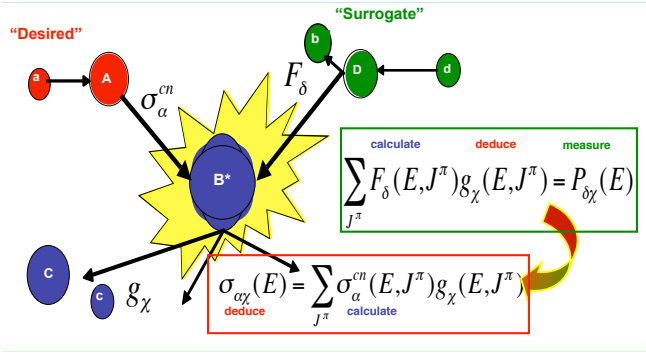

Figure 1. (color online) Surrogate idea. When the desired reaction a+A $\rightarrow$ $B^\star$ $\rightarrow$ C+c involves an unstable target A, the cross section may be deduced using theoretical modeling and experimental data from a surrogate reaction d+D $\rightarrow$ $b + B^\star$ $\rightarrow$ C+c on a stable target D. Both reactions proceed via the same compound system $B^\star$.

been various proposals for circumventing the problems associated with the use of unstable nuclei and yet to gain information about the desired nuclear reaction. One such approach is the Surrogate Method [7] shown schematically in Figure 1.

In this paper we study the reaction ^{3}He+^{157}Gd $\rightarrow$ ^{4}He+^{156}Gd* and model the formation probability of various excited states of the ^{156}Gd system within a direct reaction framework. This reaction is a surrogate for the neutron capture reaction ^{155}Gd+n $\rightarrow$ ^{156}Gd*. To study excitation energies E_{ex} of ^{156}Gd that correspond to low-energy neutron absorption by ^{155}Gd, we consider $E_{ex} > S_n = 8.536$ MeV, where S_n is the neutron separation energy for ^{156}Gd [1].

2 Mathematical Framework

Atomic nuclei exhibit a multitude of spectral phenomena, such as rotational and vibrational spectra, as well as the single-particle shell structure that explains the observed magic numbers [2,8]. Usually, rotational states of deformed even-even nuclei are modeled using simple rotational functions [2]. An extra particle is then assumed to occupy a valence single-particle state within a deformed mean-field potential. This allows one to treat the odd-even deformed nuclei within a model consisting of a rotor plus a single particle. Within this framework one can calculate cross sections for particle transfer using transition amplitudes between collective rotational states and states of a particle plus a rotor.

2.1 Energy levels of an axially-deformed rotor plus a particle system

Within the Bohr-Mottelson rotor model, an intrinsic state Φ_K of a deformed system, with axial symmetry, gives rise to a rotational band $E(J) = E_K +$

$\frac{\hbar^2}{2\mathcal{I}}(J(J+1)-K(K+1))$. Here K is the angular momentum projection onto the symmetry axis and $\mathcal{I}$ is the moment of inertia of the system, which for simplicity is assumed to be independent of K [2]. In the zero order approximation, where we neglect possible particle-core couplings, such as Coriolis coupling, the combined system of a particle/hole plus a core has an intrinsic state Φ_Ω that can be viewed as a direct product of the intrinsic state of the core Φ_K^{cor} and the single-particle/hole state ψ_ν with an angular momenta projection ν:

$$\Phi_\Omega = \psi_\nu \Phi_K^{cor},\ E_\Omega = E_K + \epsilon_\nu,$$

where $\Omega = K + \nu$ due to axial symmetry. Therefore, for the particle-plus-core system we have: $E(J) = E_\Omega + \frac{\hbar^2}{2\mathcal{I}}(J(J+1)-\Omega(\Omega+1))$.

As long as the states of interest are built from the same initial intrinsic core state, we can make perturbation adjustments to the energies to incorporate pairing and Coriolis coupling effects. Coriolis coupling $H_C = -\frac{\hbar^2}{2\mathcal{I}}(I_+ j_- + I_- j_+)$ is known to be an important interaction, where $I_\pm$ and $j_\pm$ are the ladder spin operators for the core and single particle [9–12]. It is known that the first-order perturbation to the energy is non-zero for $\Omega = \frac{1}{2}$ bands only and higher order terms are needed to obtain the energy shifts in $\Omega > \frac{1}{2}$ bands [9, 10]. We consider only one intrinsic state of the core (the ground state of the target) coupled to various neutron holes in the core. This, therefore, eliminates any Coriolis band mixing from our model. We use a phenomenological adjustment that reproduces the experimentally observed splitting between $\Omega = 0$ and $\Omega = 3$ bands in ^{156}Gd by using the experimental moment of inertia $\mathcal{I}$ needed to reproduce the $\Omega = 0$ ground state band. We have already included particle-core effects due to the Coriolis coupling, but will neglect the pairing effects. This is justified as we are considering highly excited states in ^{156}Gd with $E_{ex} > 8.5$ MeV.

2.2 Description of the single-particle states in axially-deformed nuclei

We calculate single-particle states using Woods-Saxon mean-field potential [3]:

$$V(r,R) = V_0/(1+\exp((r-R)/a))$$

For spherical nuclei R is constant and represents the position of the nuclear surface while a is a measure of the diffuseness of the potential near the surface.

We consider axially-deformed nuclei and assume quadrupole and hexapole deformation only:

$$R(\theta,\phi) = R_0\left(1+\beta_2 Y_{20}(\theta,\phi)+\beta_4 Y_{40}(\theta,\phi)\right)$$

For small deformations ($\beta \lesssim 0.3$) one can expand the Woods-Saxon potential in Taylor series. While in many cases it seems sufficient to consider only the first-order terms in the expansion [13], some single-particle states are sensitive

to small values of beta $\beta_2 \lesssim 0.3$. Proper treatment of such states needs careful considerations [4]. If β is sufficiently small, so that the Taylor expansion converges, one can re-express $V(r, R)$ in terms of spherical harmonics [14]. An alternative way is to solve numerically the Schrödinger equation for the deformed Woods-Saxon potential [15]. When comparing the single-particle energies calculated numerically to the one calculated using only first-order Taylor expansion approximation, one finds that for rare-earth nuclei (nuclei near Gd) the "Nilsson diagrams" agree for $\beta_2 \lesssim 0.1$ but start to deviate at larger deformations; in particular, there is a substantial deviation for $m_j = j$ states [14].

For our study the neutron bound states in ^{157}Gd were calculated with the WS-BETA code [15] using Woods-Saxon parameters from Ref. [16], but $\beta_4 = 0$ so that the 47^{th} neutron state ($\epsilon_{47} = -6.361$) is near the experimental neutron separation energy $S_n = 6.3598$ MeV [17], V_0=-45.1776 MeV, r_0=1.25 fm, a_0=0.65 fm, V_{ls}=19.2015 MeV, $\beta_2 = 0.29$ and $\beta_4 = 0$ [4].

3 Reaction Cross Sections for Deformed Nuclei

We employ the zero-range Distorted Wave Born Approximation (DWBA) to calculate the 1-neutron pickup reaction [5, 18, 19]. To carry out our calculations, we need optical potentials, single-nucleon wave functions, and spectroscopic factors. To calculate the distorted waves, we have used [4] an Optical Model Potential (OMP) of Wood-Saxon type, with parameters from the Reference Input Parameter Library (RIPL-2) [20–22].

For transfer reactions, which result in low-energy excitations, the correct asymptotic tail of the wave function, which is related to the neutron separation energy, is very important in neutron pickup since transfer reactions are sensitive to the nuclear surface. Using wave functions with the desired binding energy produced by adjusting the depth of the Woods-Saxon binding potential is one of the simplest and usually very successful method in calculating the reaction cross sections. In this approach one keeps the geometric factors of the binding potential fixed from systematics, but changes the depth of the potential until a state ψ with the desired binding energy is found.

3.1 Sturmian method for reaction form-factors and spectroscopic factors

We employ a Sturmian basis to determine single-particle wave functions. This approach has advantages over alternative methods. In a Sturmian basis all the basis states have the same tail as the original state that is being expanded in this basis. In order to maintain the correct asymptotic tail one has to find different wave functions and potential strengths that result in the same energy and thus the same wave function tail. The Sturmian basis method has been utilized before in transfer reactions to highly excited states in deformed nuclei [23]. The method

in [23] relies essentially on expressing the deformed potential as linear in β_2 which may not be sufficient in the case of strong deformation.

To illustrate the role of various parameters involved, we now look at the incoherent DWBA reaction cross section for a particle transfer from a deformed single-particle state ψ_ν that can be expressed in terms of transfer cross sections on spherical single-particle states ϕ_{nlj} [18, 23]:

$$d\sigma(J_i K_i \to J_f K_f; \nu) = \sum_{lj} \sum_{n} (a_\nu v_\nu c_\nu^{nlj})^2 d\sigma_{nlj}^{DW}$$

Here σ_{nlj}^{DW} are the DWBA cross section for pickup from a spherical state ϕ_{nlj}, c_ν^{nlj} are the expansion coefficients of the state ψ_ν in spherical basis states ϕ_{nlj}, v_ν represents BCS occupation number ($v_\nu^2 = n_\nu/2$) of the state ν, and a_ν is the Coriolis band mixing amplitude. The spectroscopic factor S_{lj} is often used as shorthand notation for the term $(a_\nu v_\nu c_\nu^{nlj})^2$ above. In our calculations, we actually consider the generally more appropriate coherent cross section by using super-position of basis states ϕ_{nlj} with amplitudes $a_\nu v_\nu c_\nu^{nlj}$.

In our study, the individual cross sections, for neutron transfer from a deformed state ψ_ν that results in a final state with J^π and energy E, are calculated as coherent cross sections with the code CHUCK3 [5] using the amplitudes c_{nlj}^ν times a Clebsch-Gordan coefficient and other appropriate factors [23]: $\sqrt{(1+\delta_{0,K_i K_f})/(2j+1)} \times D_0 \times c_{nlj}^\nu \times (J_f K_f | jm, J_i, K_i)$, where D_0 is the strength of the zero range transfer potential ($D_0\delta(x)$, D_0^2=18 [19]). The resulting reaction cross-sections $\sigma_\lambda(\epsilon_\nu, J^\pi)$ is defined for each single-particle state ϵ_ν . In what follows the index λ will denote the pair of labels (ϵ_ν, J^π).

4 Neutron Transfer Reaction Results

Here we present the results for the transfer reaction ^{157}Gd(^{3}He,^{4}He)^{156}Gd. After obtaining the individual cross-sections $\sigma_\lambda(\epsilon_\nu, J^\pi)$ within the Sturmian method one can consider the total cross-section $\sigma(E)$ using a smeared function, which takes into account damping effects that are not explicit in our model. Then, the compound-formation probability distributions $P(J^\pi, E)$ can also be computed.

The transfer cross sections $\sigma_\lambda(\epsilon_\nu, J^\pi)$ are for one-nucleon removal from a deformed single-particle state ψ_{ϵ_ν} from the ^{157}Gd system. The ^{157}Gd system is the core in a $K = 3/2^-$ state. We treat the final states of the ^{156}Gd system as rotational states built on the intrinsic state Ω where Ω refers to neutron holes in the core $|A = 156, \Omega >= \psi_\nu^\dagger |A = 157, K = 3/2^- >$.

In order to calculate the cross section for a one-nucleon transfer reaction to an excited state in ^{156}Gd, we first consider an intrinsic state in ^{156}Gd as a hole in the ^{157}Gd core; then we construct rotational states built on that intrinsic state.

We use simple geometric arguments to estimate the maximum angular momentum transfer to be 4; future work may relax this constraint. Therefore, one can consider a total of 12 members of the related $\Omega = |K \pm \nu|$ rotational bands to include all possible excitations with $J < 8$. Thus, the relevant states are: $|^{156}Gd, \Omega = |K \pm \nu| >= \psi^{\dagger}_{\pm\nu}|^{157}Gd, K = 3/2^{-} >$.

$$E(J^{\pi}; \Omega = |K \pm \nu|) = \epsilon_0 - \epsilon_{\nu} + \frac{\hbar^2}{2\mathcal{I}}(J(J+1) + \delta_{\pm})$$

Here ϵ_0 is used to set the ground state energy of ^{156}Gd to zero, and $\delta_{\pm}$ is the energy shift of the $\Omega = K + \nu$ state relative to the $\Omega = |K - \nu|$ state. Thus if we set $\delta_{-} = 0$ for $\Omega = |K - \nu|$ then $\delta_{+} = 2cK\nu$ for $\Omega = K + \nu$ states. We always keep Ω, ν, and K positive when we use them as labels for the states.

By fitting the first four excited states of the $\Omega = 0^{+}$ ground state band, the moment of inertia is fixed to be $\hbar^2/2\mathcal{I} = 13.59$ KeV for the rotational bands in ^{156}Gd. The $c = 17.741$ coefficient for the Coriolis energy shift of the related $\Omega = 3^{+}$ band was chosen to reproduce the excitation energy of the 3^{+}_{1} state. The value of c is about 1.65 times the ratio of the moments of inertia $\mathcal{I}_{||}/\mathcal{I}_{\perp}$ for rigid ellipsoid with $\beta = 0.29$. This way were are within few keV of the experimental values for the 0^{+} ground state band and the 3^{+} band [4].

4.1 Neutron pickup cross sections

To be able to use existing reaction codes, we have to expand the deformed single-particle states in a spherical basis. Here we consider the Sturmian approach by using Sturmian spherical basis states. We calculate the spectra of a deformed Woods-Saxon potential using standard bound-states technique and employ the code WSBETA [15]. Then for each state ψ_{ν} with energy ϵ we find all the Sturmian spherical basis states (zero deformation) $\phi_{\epsilon nlj}$ with nlj labels as for a spherical harmonic oscillator up to the N_{max} oscillator shell. These basis states are constructed with the reaction code DWUCK4 [19]. For a fixed ϵ and nlj labels the code finds a scaling factor for the original spherical potential such that $\phi_{\epsilon nlj}$ is a bound state of this new potential. This scaling factor is then used to recompute the state $\phi_{\epsilon nlj}$ within the WSBETA code in the same basis where the deformed state ψ_{ν} has been computed. The expansion amplitudes c^{nlj}_{ν} are then calculated [4] and passed to the reaction code CHUCK3 [5], which has the ability to add the c^{nlj}_{ν} amplitudes coherently.

The cross sections that one can calculate within the presented framework correspond to sharp final states. In reality there are widths associated with the single-particle states as well as with the final states. In order to produce a smooth total cross section as a function of the excitation energy of the ^{156}Gd system we consider a smearing distribution function of Lorentzian type:

$$\rho_{\nu}(E) = \frac{1}{2\pi}\frac{4\Gamma}{4(E - E_{\nu})^2 + \Gamma^2},$$

with $\Gamma = a + bE$ and define a smooth $\sigma(E)$ cross-section [23]:

$$\sigma(E) = \sum_{\lambda} \rho_{\lambda}(E)\sigma_{\lambda}$$

The smeared cross sections, introduced above, can be used to determine a smooth probability to excite a state with quantum numbers J^{π}:

$$P(J^{\pi}; E) = \frac{1}{\sigma(E)} \sum_{\lambda} \delta_{J,J_{\lambda}} \delta_{\pi,\pi_{\lambda}} \rho_{\lambda}(E)\sigma_{\lambda}$$

In Figure 2 we show the $P(J^{\pi}; E)$ distributions that are of interest to the surrogate method through direct neutron pickup via 42 MeV ^{3}He on ^{157}Gd target. We find that all final spins from $J = 0$ to $J = 8$ are populated. The calculated formation probability P(J$^{\pi}$,E) resembles Gaussian distributions with magnitudes, centroids, and width that are different for positive and negative parity states. The parity asymmetry in the $P(J^{\pi}, E)$ distribution can be tracked back to the neutron single-particle states and their energies. There is a 2 MeV gap between the single-particle states with energy -16.81 MeV and -14.66 MeV that results in absence of positive-parity states in the 10 MeV excitation energy region [4]. The results are to be considered a first estimate for the spin-parity distribution. A more comprehensive treatment would need to relax the geometric estimate of an upper limit for the angular momentum transfer. Also, recent work [24] has demonstrated that two-step reaction mechanisms can play an important role in transfer reactions that populate highly-excited states (above a few MeV).

5 Concluding Remarks

The present computational method is a first step to particle pick-up reactions in deformed and strongly deformed systems. Recent work on spherical systems has shown that pickup reactions which create highly-excited states, have important contributions from two-step processes, such as pickup followed by inelastic excitation and vice versa. The present work needs to be extended to include those contributions.

Our calculations show that within the assumptions outlined here, the one-step contribution to the reaction ^{3}He+^{157}Gd $\rightarrow$ ^{4}He+^{156}Gd* has a smoothly-varying formation probability $P(J^{\pi}, E)$ within a wide energy range relevant to the desired reaction ^{155}Gd+n $\rightarrow$ ^{156}Gd*. Thus, given an experimental input on the decay probability $P_{\delta\chi}$ into an exit channel χ within the surrogate formation channel δ, one should in principle be able to determine $g_{\chi}(J^{\pi}, E)$ using the approach outlined in Refs. [7, 24].

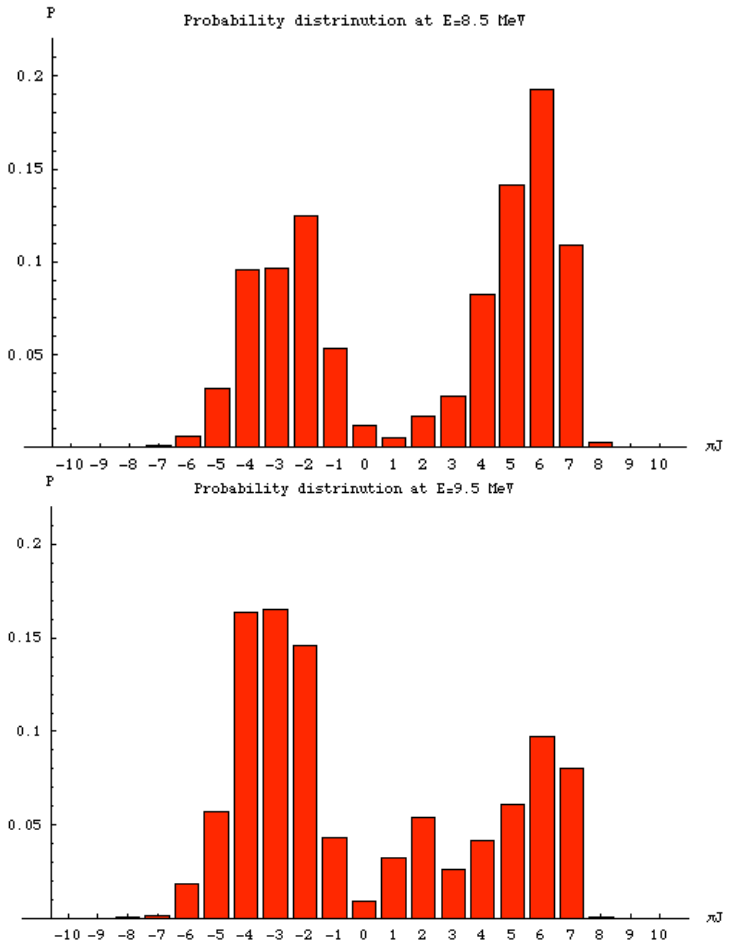

Figure 2. (color online) $P(J^\pi; E)$ distributions for energies near the neutron separation energy in ^{156}Gd. Top graph for $E = 8.5$ MeV and bottom $E = 9.5$ MeV (using $\Gamma = 0.01 + 0.01E$ for the smearing function). The sign of the horizontal coordinate corresponds to the parity π and its magnitude gives J.

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