Rotational-vibrational Description of Nucleon Scattering on Actinide Nuclei Using a Dispersive Coupled-channel Optical Model

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(Dated: February 25, 2014)

Tamura's coupling formalism has been extended to consider low-lying rotational bands built on vibrational (single-particle) band heads in well-deformed even-even (odd) actinides. These additional excitations are introduced as a perturbation to the underlying rigid rotor structure that is known to describe well the ground state rotational band of major actinides. Coupling matrix elements needed in extended Tamura's formalism are derived for both even-even and odd actinides. Employed dispersive optical model (DCCOMP) replaces the incident proton energy E_p (for proton induced reactions) by the equivalent Coulomb subtracted energy in all potential terms including both the imaginary and real potentials with the corresponding dispersive corrections. Therefore, the optical potential becomes fully symmetric for protons and neutrons. This potential is used to fit simultaneously all the available optical experimental databases (including neutron strength functions) for nucleon scattering on ^{238}U and ^{232}Th (even even) nuclei. Quasi-elastic (p,n) scattering data to the isobaric analogue states of the target nuclei are also used to constrain the isovector part of the optical potential. Derived Lane-consistent DCCOMP is based on coupling of almost all levels below 1 MeV of excitation energy. The ground state, octupole, beta, gamma and non-axial rotational bands are considered for even nuclei, and rotational bands built on single-particle levels – for odd nuclei. Application of derived potential to odd targets based on a new coupling scheme is foreseen.

I. INTRODUCTION

High accuracy requirements were placed on neutron inelastic cross-sections on the major component of nuclear reactor fuel ^{235,238}U in the whole energy range up to 20 MeV by the OECD/NEA WPEC SG-26 [1]. The improvement of cross sections and emission spectra and reduction of their uncertainties for neutron induced reactions on both ^{235}U (fissile) and ^{238}U (fertile) actinides are important issues that should initiate new theoretical studies. Using the optical model one can calculate not only total, elastic and reaction cross sections, but also transmission coefficients for the statistical and pre-equilibrium model calculations. Thus, a phenomenological optical model potential that is capable of describing with high accuracy available scattering data for both even-even and odd targets over a wide energy range is essential to meet data needs mentioned above.

II. DISPERSIVE OPTICAL MODEL POTENTIAL WITH FULL COUPLING

Detailed formulation of the dispersive coupled-channel optical model potential (DCCOMP) has been presented in our previous works [2–5]; a brief summary is given next. In the present work we focus on improving the model of nuclear structure used in coupled-channel calculations, especially for odd-mass targets.

A. The Dispersive Nature of DCCOMP

Under favorable conditions of analyticity in the complex E-plane the polarization correction ΔV to the smoothly energy-dependent Hartree-Fock (HF) term, $V_{HF}(\mathbf{r}, E)$ can be constructed from the knowledge of the imaginary part W on the real axis through the dispersion relation

$$\Delta V(\mathbf{r}, E) = \frac{\mathcal{P}}{\pi} \int_{-\infty}^{\infty} \frac{W(\mathbf{r}, E')}{E' - E} dE' \ , \qquad (1)$$

where $\mathcal{P}$ stands for the principal value of the integral. To simplify the problem, the geometry of the imaginary terms of the DCCOMP are usually assumed to be energy-independent and they are expressed in terms of a Woods-Saxon function. In such case, the radial functions factorize out of the integrals and the energy dependence is completely accounted for by two overall multiplicative strengths $\Delta V(E)$ and $W(E)$. Both of these factors contain, we note, volume and surface contributions. A similar assumption is used for the spin-orbit potential where the real spin-orbit strength consists of a term which varies

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slowly with energy $V_{SO}(\mathbf{r},E)$, plus a correction term, $\triangle V_{SO}(\mathbf{r},E)$, which is calculated using a dispersion relation (1).

B. Lane Consistency of the DCCOMP and Excitations of the Isobaric Analog States (IAS)

Our current formulation for proton induced reactions replaces the incident proton energy E_p by the equivalent Coulomb subtracted energy in all potential terms including both the imaginary and real potentials making the potential fully symmetric for protons and neutrons, and therefore Lane consistent [6]. Using this fully symmetric formulation we included the quasi-elastic scattering on the isobar analogue states (IAS data) of the target in the fitting. IAS data proved critical to consistently estimate the strength of the isovector component of the DCCOMP.

C. Nuclear Shapes and coupling potential

While the nuclear structure of even-even actinides below 500 keV corresponds to a rigid rotor, above 500 keV several vibrational bands are observed in the excited spectrum that have to be included in the coupling scheme [7]. For odd nuclei there are rotational bands built on low-energy single-particle bandheads. We propose new band couplings derived from the soft-rotor description [8] of the low-lying levels of actinides, but consistent with the rigid-rotor behaviour at low excitation energies. The Taylor expansion is made by assuming small dynamical departures (axial and non-axial quadrupole and octupole) from a larger static axial equilibrium quadrupole deformation (β_{20}), as given by Eq.(4) in Ref.[9].

1. *Even-even nuclei*

By performing a multipole expansion it is possible to obtain the coupled-channel matrix elements needed in reaction calculations, where effective values of the dynamic deformations are multiplied by the relevant reduced matrix elements, which contain the nuclear structure information. Using Tamura's notations [10, 11], these couplings for even-even targets are given by Eq. (7) in Ref.[9]

In Fig. 1 the calculated ratio between the difference and the averaged total cross section for ^{238}U and ^{232}Th nuclei is plotted and compared with experimental data [12]. An excellent agreement is achieved with the current DCCOMP that couples 15 levels for neutrons, even a better description than the already nice agreement observed for a dispersive RIPL 2408 potential (where only the ground-state rotational band is coupled) [3, 5]. Non-dispersive potential RIPL 2601 by Soukhovitskii and coworkers is out of phase [13].

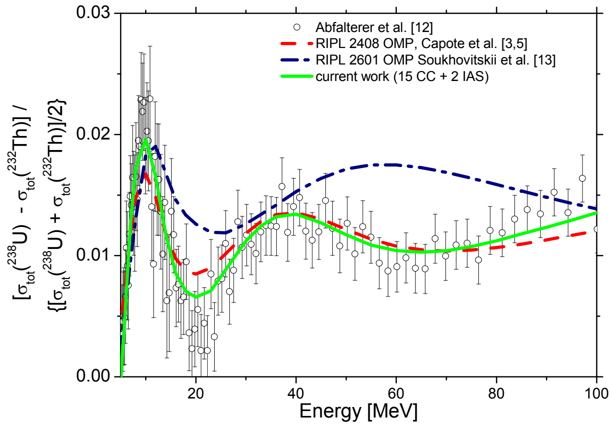

FIG. 1. Figure of merit: energy dependence of measured total cross section ratio $[\sigma_{tot}(^{238}\text{U})$- $\sigma_{tot}(^{232}$ Th)] /{$[\sigma_{tot}(^{238}\text{U})$+ $\sigma_{tot}(^{232}$ Th)]/2}.

2. *Extension to odd-A nuclei*

The situation for neutron scattering on odd actinides is even more complex, as no pairing gap exists due to the odd particle, therefore low-lying excited states are dominated by bands built on single-particle (1QP) states. Such rotational bands are observed at very low excitation energies (e.g. the $K = 1/2+$ band observed at 0.0001 keV for ^{235}U), and are strongly excited in neutron induced reactions. Therefore for odd nuclei, we may neglect rotational bands built on vibrational bandheads, and only consider rotational bands built on 1QP states. In this contribution we also neglect the interaction of the unpaired nucleon with the even-even deformed core.

Following Refs.[14, 15], we assume that the odd-nucleon eigenfunctions of the single-particle Hamiltonian H_p can be expanded in a complete spherical basis $\chi_\nu = \sum_{j\Omega} c_{j\Omega}\ \chi^j_\Omega$, where χ^j_Ω are the spherical-basis single-particle eigenfunctions, being j, Ω the total angular momentum of the unpaired nucleon, and its projection on the nuclear axis. The total wave function can be expressed as:

$$\psi_{IM\pi,\{\tau\}} = \sqrt{\frac{2I+1}{16\pi^2}}\times \qquad (2)$$
$$\sum_K {}'C_K \left[D^I_{MK}\chi_\nu + (-1)^{I-1/2+\pi} D^I_{M-K}\chi_{-\nu}\right] =$$
$$\sqrt{\frac{2I+1}{16\pi^2}}\times$$
$$\sum_K {}'C_K \sum_{j\Omega} {}'c_{j\Omega} \left[D^I_{MK}\chi^j_\Omega + (-1)^{I-j+\pi} D^I_{M-K}\chi^j_{-\Omega}\right]$$

where $\pi = 0(1)$ denotes the positive (negative) parity, and τ stands for additional quantum numbers; C_K is the K-mixing coefficient; and the sums over K and Ω are restricted to their allowed values. Following the same method used for the even-even nucleus, we derive for odd-

A nuclei the generalization of Eq. (7) in Ref.[9] by including one additional term that corresponds to octupole (axial and nonaxial) deformations:

$$[\beta_{33}]_{eff} \sum_{\lambda=3,5,7} \left[\tilde{v}_\lambda^{(3)}(r)\right]_3 \times \quad (3)$$
$$< I, \{\tau\} || \left(D^\lambda_{;3} - D^\lambda_{;-3}\right) || I', \{\tau'\} > A(lI; l'I'; \lambda J)$$

where $\left[\tilde{v}_\lambda^{(3)}(r)\right]_3$ is the generalization of the radial factors in Refs.[9, 11]. The reduced matrix elements describing the channel couplings for $\Delta K = 0, 2, 3$ are given by

$\Delta K = 0$ couplings ($\lambda = even$):

$$< I, \{\tau\} || D^\lambda_{;0} || I', \{\tau'\} >= \quad (4)$$
$$\sqrt{2I'+1} \sum_K |C_K|^2 \ \alpha(K,K) \ C^{I,K}_{I',K;\lambda,0}$$

where $C^{I,K}_{j_1,m_1;j_2,m_2}$ is a Clebsch-Gordan coefficient linking the angular momentums I, j_1, j_2 and their projections $K = m_1 + m_2$, $\alpha(K,K)$ is the $K = K'$ case of the more general expression

$$\alpha(K,K') = \sum_{j\Omega}{}' |c_{j\Omega}|^2, \quad (5)$$

where Ω is restricted to the allowed values for given K and K' .

$\Delta K = 2$ couplings ($\lambda = even$):

$$< I, \{\tau\} || \left[D^\lambda_{;2} + D^\lambda_{;-2}\right] || I', \{\tau'\} >= \sqrt{2I'+1} \times \quad (6)$$
$$\sum_{KK'}{}' \ C_K C_{K'} \ \alpha(K,K') \ \{C^{I,K}_{I',K';\lambda,2} + (-1)^{I'-1/2} C^{I,K}_{I',-K';\lambda,2}$$
$$+ (-1)^{I-1/2} C^{I,-K}_{I',K';\lambda,2} + (-1)^{I-I'} C^{I,-K}_{I',-K';\lambda,2}\}$$

where $\alpha(K,K')$ is given by Eq.(5), and $K \pm K'$ is even.

$\Delta K = 3$ couplings ($\lambda = odd$):

$$< I, \{\tau\} || \left[D^\lambda_{;3} - D^\lambda_{;-3}\right] || I', \{\tau'\} >= \sqrt{2I'+1} \times \quad (7)$$
$$\sum_{KK'}{}' C_K C_{K'} \ \alpha(K,K') \{C^{I,K}_{I',K';\lambda,3}$$
$$+ (-1)^{I'-1/2} C^{I,K}_{I',-K';\lambda,3} + (-1)^{I-1/2} C^{I,-K}_{I',K';\lambda,3}$$
$$+ (-1)^{I-I'} C^{I,-K}_{I',-K';\lambda,3}\}$$

where $\alpha(K,K')$ is given by Eq.(5), and $K \pm K'$ is odd.

III. CONCLUSIONS

We have derived coupling-matrix elements for the vibrational-rotational description of even-even (odd) well-deformed nuclei (e.g. fertile and fissile uranium isotopes). For odd-nuclei we neglected both the vibrational excitations and the interaction of the unpaired nucleon with the deformed even-even core. A full Lane-consistent formalism is used that includes Coulomb energy shifts in all potential terms for protons. We have shown that a derived Lane-consistent dispersive phenomenological optical model is capable of predicting nucleon induced cross sections on even-even actinide nuclei coupling almost all collective levels below 1 MeV. The derived potential is valid from 1 keV to 200 MeV and gives an excellent description of total cross section differences of ^{238}U and ^{232}Th. Testing of the derived potential with new coupling matrix elements on fissile (odd) actinides is in progress.

Acknowledgements: This work was funded by the Spanish Ministry of Economy and Competitivity under Contract FIS2011-28738-C02-01 and the International Science and Technology Center under contract B-1804.

[1] M. Salvatores (*coord.*), OECD/NEA WPEC Subgroup 26, NEA Tech. Rep.**6410** (2008).
[2] E.Sh. Soukhovitskiĩ *et al.*, Phys. Rev. C**72**, 024604 (2005).
[3] R. Capote, E.Sh. Soukhovitskiĩ, J.M. Quesada and S. Chiba Phys. Rev. C**72**, 064610 (2005).
[4] J.M. Quesada, R. Capote, E.Sh. Soukhovitskiĩ, S. Chiba, Phys. Rev. C**76**, 057602 (2007).
[5] R. Capote *et al.*, J. Nucl. Sci. Technol. **45**, 333 (2008).
[6] A.M. Lane, Phys. Rev. Lett. **8**, 171 (1962).
[7] T. Kawano, N. Fujikawa and Y. Kanda, Technical Report INDC(JPN)-169 (1993).
[8] E.Sh. Soukhovitskiĩ, S. Chiba, R. Capote, J.M. Quesada *et al.*, JAERI Tech. Rep. JAERI-Data/Code 2008-025, Japan (2008).
[9] J.M. Quesada, E.Sh. Soukhovitskiĩ, R. Capote and S. Chiba, EPJ Web of Conf. **42** (2013) 02005.
[10] T. Tamura, Rev. Mod. Phys. **17**, 679–708 (1965).
[11] T. Tamura, Nuclear Physics A **73**, 241 (1965).
[12] W.P. Abfalterer *et al.*, Phys. Rev. C**63**, 044608 (2001).
[13] E.Sh. Soukhovitskiĩ *et al.*, J. Phys.G: Nucl. Part. Phys.**30**, 905 (2004).
[14] A. Bohr, Mat. Fys. Medd. Dan. Vid. Selsk. **26**, No. 14 (1952)
[15] K. Hecht and G. Satchler, Nucl. Phys. **32**, 286-318 (1962).