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A SIMPLIFIED UNIFIED HAUSER-FESHBACH /PRE-EQUILIBRIUM MODEL FOR CALCULATING DOUBLE DIFFERENTIAL CROSS SECTIONS†

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ABSTRACT

A unified Hauser-Feshbach/Pre-Equilibrium model is extended and simplified. The extension involves the addition of correlations among states of different total quantum numbers (J and J') and the introduction of consistent level density formulas for the H-F and the P-E parts of the calculation. The simplification, aimed at reducing the computational cost, is achieved mainly by keeping only the off-diagonal terms that involve strongly correlated $2p$-$1h$ states. A correlation coefficient is introduced to fit the experimental data. The model has been incorporated into the multistep H-F model code TNG. Calculated double differential (n, xn) cross sections at 14 and 25.7 MeV for iron, niobium, and bismuth are in good agreement with experiments. In use at ORNL and JAERI, the TNG code in various stages of development has been applied with success to the evaluation of double differential (n, xn) cross sections from 1 to 20 MeV for the dominant isotopes of chromium, manganese, iron, nickel, copper, and lead.

INTRODUCTION

Hauser-Feshbach/pre-equilibrium model codes have been widely used for calculating neutron-induced reaction cross sections from a few keV to several tens of MeV. The ability of the H-F model, based on the random phase approximation, in calculating angular distributions for the equilibrium part is well-established. Plyuiko[1] has attempted to unify the two models for the purpose of calculating angular distributions for the P-E part with the same components as for the H-F part by allowing fully correlated phases in the partial waves forming states of a fixed total angular momentum (J) in the first pre-equilibrium stage (n_0). We have found it necessary to allow cross terms involving different J's and to change the full correlation into partial correlation by introducing a correlation coefficient. Deviations in the spin distributions in the composite nucleus in the P-E stage from the

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H-F stage are accounted for and lead to enhanced peripheral emission in the pre-equilibrium stage. The model is then simplified by removing many second order terms. Good agreement of calculated double differential (n, xn) cross sections with experimental data for two incident neutron energies and for both even-even and odd-A targets over a wide mass range was obtained. In the calculations for the odd-A targets, the target spin was assumed to be inactive in the P-E stage but active as usual in the H-F stage.

THE UNIFIED FORMULA

The double-differential cross section due to both the H-F and P-E models, derived by Plyuiko[1] and here modified by adding a summation over J', is given by

$$d^2\sigma(a,b;J_x)/dE_b d\Omega = k\sum_L (D_L + B_L)P_L(cos\ \theta), \tag{1}$$

with

$$D_L = \sum (-1)^{j_a - j_b} Z_a Z_b T_a T_b \sum_{n,\Delta n=2} f(n,U,J,\Pi)\rho(n-n_b, U_y, J_y, \Pi_y), \tag{1a}$$

and

$$B_L = \sum{}' (-1)^{j_a - j_b} Z'_a Z'_b (T_a T'_a T_b T'_b)^{\frac{1}{2}} [f(n_0,U,J,\Pi) f(n_0,U,J',\Pi')]^{\frac{1}{2}}$$

$$\rho(n_0 - n_b, U_y, J_y, \Pi_y), \tag{1b}$$

where

a = the incident particle
x = the target nucleus
b = the outgoing particle
y = the residual nucleus
$k = \lambda_a^2/[4(2J_a+1)(2J_x+1)]$
Z = Z coefficients defined in ref. 2; e.g. $Z'_a = i^{\ell_a - \ell'_a - L} Z(\ell_a J \ell'_a J'; j_a L)$
T = optical model transmission coefficients; e.g. $T'_b = T(E_b, j_b, \ell'_b)$
f = pre-equilibrium weighting function $= \tau(n,U,J,\Pi)Q_b(n)/[h\rho(n,U,J,\Pi)]$
$\tau = \int_0^\infty P(n,U,J,\Pi,t)dt$ = mean lifetime of states with exciton number n, excitation energy U, spin J, and parity Π
P = occupation probability of exciton states
Q = a factor defined by Kalbach[3] for neutron-proton distinguishability (not used by Plyuiko but added here to enhance the applicability of the model)

$\sum$ = sum over J, Π, J_y, Π_y, j_a, j_b, ℓ_a, and ℓ_b

$\sum'$ = sum over J, Π, J', Π', J_y, Π_y, j_a, j_b, ℓ_a, ℓ'_a, ℓ_b, ℓ'_b with the restriction $J \neq J'$, and/or $\ell_a \neq \ell'_a$, and/or $\ell_b \neq \ell'_b$.

The prime is used to denote a different value of the unprimed quantity. The quantities without a subscript, such as n, U, J, and Π, are for the composite nucleus. The remaining variables are recognizable and are defined elsewhere[4].

The reason for adding the sum over J' is now explained. The assumption that states with different total angular momenta in the composite nucleus are not correlated was not explained by Plyuiko. The assumption probably originated from a desire for saving computing effort. However, this assumption cannot be justified. For example, the assumption breaks down for an alpha-particle induced reaction on even-even targets. Since the incident channel spin for such a reaction is zero, none of the incoming partial waves can interfere for a fixed J to generate any odd Legendre coefficients. Consequently, all alpha-particle-induced reactions on even-even targets would have to emit particles symmetrically about 90 degrees in the center-of-mass frame, a prediction contrary to forward-peaked angular distributions commonly observed in the pre-equilibrium energy ranges. Therefore, we added the summation over J' throughout Plyuiko's derivations. By removing the sum over J' and Π' in Eq. (1b) and by replacing J' and Π' with J and Π in $f(n_0, U, J', \Pi')$, Eq. (1) becomes the original Plyuiko's formula. Unfortunately, the newly added summation much increased the necessary computation. To compensate, other simplifications are sought, as discussed next.

SIMPLIFYING APPROXIMATIONS

Three symplifying approximations were made and are summarized below. The third one has to do only with an odd-A or odd-odd target.

1. The deviations of the spin and parity distributions in the pre-equilibrium weighting function f from the equilibrium distributions are considered only for the initial exciton states ($n_0 = 3$ in the present calculations). These n_0 spin and parity distributions are taken to be an average of those at $t = 0$ and $t = T$ (the equilibration time). The deviations of these distributions from the equilibrium distributions lead to an enhancement of pre-equilibrium emission from large J-states (peripheral emission). For $n > n_0$, the usual H-F spin and parity distributions are used, saving a lot of computations for the minor components. Advanced treatments of pairing correction[5] and pairing-corrected spin distributions[6] for the particle-hole level densities are adopted to ensure that the unified model does not required any more level density parameters as already required by the H-F model.

2. Only those terms in Eq. (1) that can contribute to the P_0 and P_1 Legendre coefficients are kept. This approximation represents a first

order relaxation of the RPA approximation used for the H-F model and leads to very large savings in computation. A simple way to think of the approximation is as follows. Those terms that can give P_0 are the usual H-F terms (the diagonal terms), therefore kept, while those that can give P_1 (the near-diagonal terms) approximately represent the "memory" of the incident direction by the outgoing particle in a strongly localized pre-equilibrium collision. The latter is weighted by a correlation coefficient (between 0 and 1) to account for a partial dissipation of this memory.

3. For an odd-A target, the odd nucleon and its spin have little chance of participation in the first pre-equilibrium stage but will take part in the H-F stage. This consideration is accounted for by calculating the P-E and the H-F components separately, setting the true target spin to zero in the pre-equilibrium run. The TNG code was programmed to do this.

VALIDATION OF THE MODEL

Selected double differential (n, xn) data at 14 and 25.7 MeV for ^{56}Fe, ^{93}Nb, and ^{209}Bi were used to test the present model. This choice provided two incident neutron energies, a wide mass range, and both even-even and odd-A targets. Extensive numerical experiments were performed to check the above simplifying approximations. Good agreement with data was obtained with a constant correlation coefficient of 0.5 and a standard set of optical model, level density, and P-E parameters. A detailed description of this work[4] is available upon request.

The same correlation coefficient and parameters as above were applied to the Blind Pre-equilibrium Benchmark[7] for neutron emission from 25.7-MeV incident neutrons on ^{184}W. (See also proceedings of this meeting for the many interesting contributions to this intercomparison.)

Our contribution to the ^{93}Nb intercomparison[8] was made with an earlier version of the code before the third approximation was implemented. The calculation was done by setting the target spin to zero for both the P-E and H-F parts. This, of course, led to less valid results for the H-F part, which, in turn, affected the P-E part of the calculation because the two competed. However, the results remained satisfactory in comparison with the widely spread data. Our new calculation[4] yielded better agreement.

APPLICATION OF THE TNG CODE

The model described here has been applied to the ENDF/B-VI evaluations of iron and lead. Preliminary versions of the code have been used for the chromium, manganese, nickel, and copper evaluations with considerable success. Reports, preprints, or summaries on these are available upon request. However, we encountered a difficulty in the lead evaluation which is described below.

As shown in Fig. 1, the neutron emission spectrum from 14-MeV Pb(n, xn) reaction has a flat portion for E'_n between 6 and 9 MeV. This

E'_n range is usually dominated by the P-E reaction which cannot yield a flat spectrum, a spectrum possible only in collective reactions. To meet our ENDF/B-VI schedule, we tentatively added a constant state density (a parameter) to the $1p$-$1h$ state density for the residual nucleus, thus flattening the P-E spectral shape. The result is shown in Fig. 1, together with the ENDF/B-V evaluation and the recent data of Takahashi[9]. This approach is unfounded and is an area we plan to improve in the near future. Fortunately, the double differential cross-section data[9-11], shown in Fig. 2, are still well reproduced with the global correlation coefficient of 0.5.

The same difficulty encountered in the lead calculation also exists (see proceedings of this meeting) in our ^{184}W calculation[7]. Strong collective excitation (vibration for Pb and rotation for W) is expected in each case and a simple approximation for such an excitation is desirable. In the calculation shown in Fig. 1, DWBA results for many discrete levels were already included but there is still too big a gap between the collective range and the H-F/P-E range.

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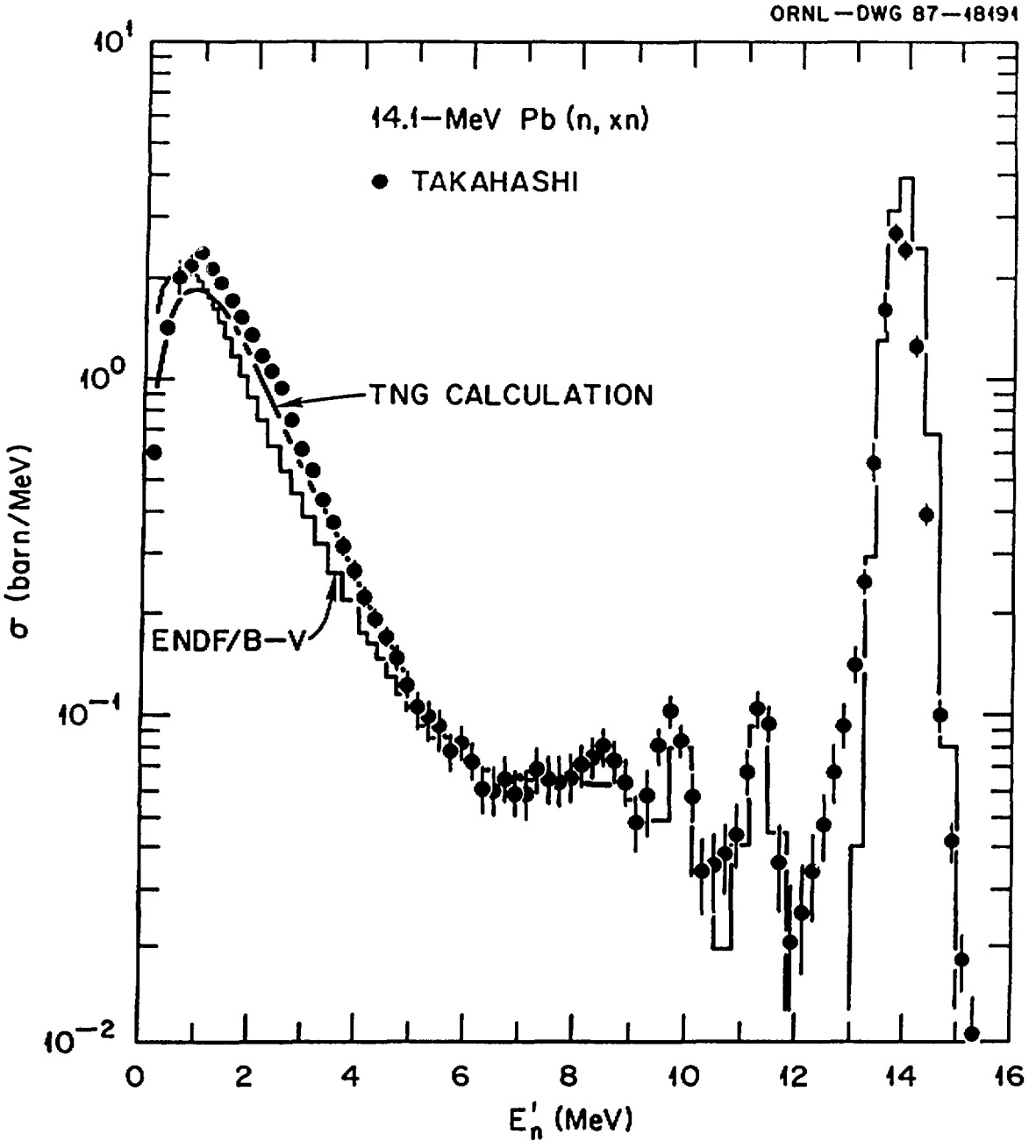

Fig. 1. Neutron emission spectrum from 14.1-MeV Pb(n, xn) reaction.

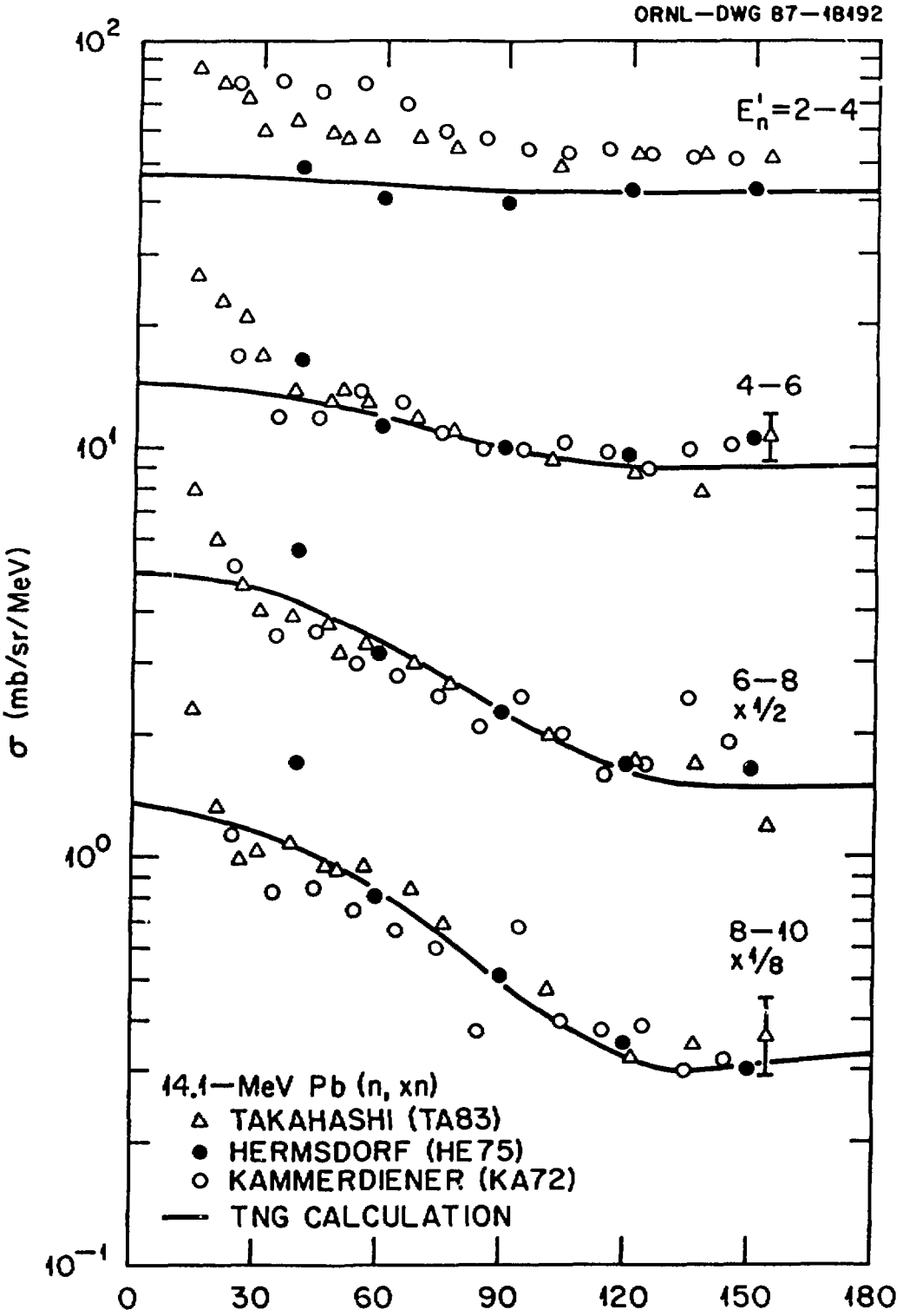

Fig. 2. Double differential neutron-emission cross sections from 14.1-MeV Pb(n, xn) reaction.

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