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The Theory of Partial Fusion

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Abstract. A theory of partial fusion is used to calculate the competition between escape (breakup) and absorption (compound-nucleus production) following a deuteron-induced transfer of one neutron to a heavy nucleus at energies above the neutron escape threshold. Preliminary calculations are shown to yield excellent results for the competition between neutron absorption and neutron escape when deposited on actinides at energies up to 3 MeV.

1. The problem

A difficulty in reaction theory arises when there is a simultaneous absorption of one part of a composite system: we need to be able to distinguish complete and no fusion from incomplete fusion. After the absorption of one fragment, we want to still follow the evolution of remaining part(s), in order to see whether it escapes (yielding incomplete fusion) or fuses with the target (yielding complete fusion). When it may escape, we want to predict its angular scattering amplitudes,

Experiments [1], for example, have measured protons from (d,p) reactions on actinides, both with and without coincidence with fission events. The ratio $\sigma(d,pf)/\sigma(d,p)$ between these cross sections can be taken as an estimate of the fission probability at a neutron energy determined from the measured proton energies by $E_n = E_{tot} - 2.226 \text{ MeV} - E_p$. However, using fission probabilities from ²³⁹Pu(d,pf) does not give correct (n,f) cross sections if it is assumed that all (d,p) transfer reactions lead to compound nucleus formation. From Fig. 1, we see that the results can differ from evaluated fission probabilities by up to 40% even at 2 MeV of equivalent neutron energy.

This is precisely the kind and direction of difference we find with a theory of partial fusion. The observed $\sigma(d,p)$ rate includes escape (breakup) as well as absorption (compound-nucleus production), so the denominator in $\sigma(d,pf)/\sigma(d,p)$ is too large.

2. Theory

There have been attempts to extend standard few-body reaction theory to describe more general outcomes: by Udagawa and Tamura [2], of Kerman and McVoy [3] (based on [4]), and of Baur and Trautman [5], as well as a proposal of my own [6], but these give different results[7].

Now I follow the theory of Austern [8] that sums over the final states of just one (neutron) particle of a few-body system (eg. deuteron), and show how partial sums of the cross sections to those states can be expressed as integrals of the imaginary component of that particles optical potential. In this derivation we need not make any first-order approximations in the entrance channel wave functions, and can ensure post-prior equivalence for the transfer matrix elements.



Figure 1. Fission probabilities for neutrons incident on ²³⁹Pu. Comparison of two surrogate experiments with probability from the ENDF/B.VII evaluation (the ratio of the fission cross section to the reaction cross section). The energy scale is E_n : the continuum neutron energy in ²⁴⁰Pu^{*}.

3. Calculations

The normal (d,p) formalism calculates the cross sections for a neutron being captured into a bound state around the target, with the proton escaping and being measured. The *T*-matrix for this process has the standard form of

$$T_{dp}(\mathbf{k}_p) = \langle \psi^{(-)}(r_p; \mathbf{k}_p) \phi(r_n) | V | \phi_d(\mathbf{r}) \Psi^{(+)}(\mathbf{R}) \rangle, \qquad (1)$$

where $\phi(r_n)$ is the neutron final state in real potential, $\phi_d(r)\Psi^{(+)}(R)$ is incoming deuteron wave function, and V is the transfer interaction (post or prior). Using partial wave expansions, this integral can be written as sums of L-dependent matrix elements like

$$T_{L_n L_p}^{L_d}(k_p) = \langle \psi_{L_p}^{(-)}(r_p; k_p) \phi_{L_n}(r_n) | V | \phi_d(r) \Psi_{L_d}^{(+)}(R) \rangle.$$
(2)

Now, however, the neutron is in a complex potential $V(r_n) - iW(r_n)$. Here, the $-iW(r_n)$ term describes the loss of flux to CN resonances, which is the 'spreading' into CN resonances. This is the same as the reaction cross section for neutrons incident by themselves, or, within a deuteron-nucleus reaction, a partial fusion cross section.

In order to calculate this partial fusion, we make 'proton bin' wave function $\xi^{(-)}(r_p; \overline{k_p})$ by averaging the proton outgoing waves over small sections $[k_1, k_2]$ of momentum space:

$$\xi_{L_p}^{(-)}(r_p; \overline{k_p}) = \sqrt{\frac{2}{\pi(k_2 - k_1)}} \int_{k_1}^{k_2} \psi_{L_p}^{(-)}(r_p; k_p) dk_p.$$
(3)

This bin wave function is square-integrable, and hence can be used as the final captured state in an DWBA-like matrix element. This allows transfer cross section calculations to converge without the use of Vincent-Fortune [9] complex continuations for asymptotically large radii.



Figure 2. Results for the reaction $d + {}^{239}Pu \rightarrow p + {}^{240}Pu$ at $E_d = 15$ MeV. The left plot shows the partial fusion cross sections as a function of energy across the neutron escape threshold, for different spins L_N of the absorbed neutron. The right plot shows that partial fusion (black) and breakup escape (red) cross sections as a function of partial wave L_p of the outgoing proton.

Now, to find the propagation of the neutron in an optical potential after transfer, we solve an inhomogeneous equation with source term:

$$[H_n - E_n]\psi_{L_pL_d}^{L_n}(r_n; \overline{k_p}) = \langle \xi_{L_p}^{(-)}(r_p; \overline{k_p}) | V | \phi_d(r) \Psi_{L_d}^{(+)}(R) \rangle.$$

$$\tag{4}$$

The CN production cross section, integrating over all proton angles (summing over all L_p), is then

$$\sigma_{\rm CN}^{L_n}(\overline{k_p}) = 4\pi \frac{2}{\hbar v_d} \sum_{L_d L_p} (2L_d + 1) \int_0^\infty |\psi_{L_p L_d}^{L_n}(r_n; \overline{k_p})|^2 W(r_n) dr_n, \tag{5}$$

which retains its dependence on the proton energy $E_p = \hbar^2 \overline{k_p}^2 / 2\mu_p$.

4. Results

Figure 2 shows our first results, for exit cross sections integrated over all proton angles, from Eq. (5). Later work will use a full partial wave expansion of Eq. (1) and hence give the CN cross section as a function of both the magnitude and direction of \mathbf{k}_p , the outgoing proton momentum. The left plot shows calculated values of $\sigma_{\mathrm{CN}}^{L_n}(k_p)$ plotted as function of neutron continuum energy $E_n = E_{\mathrm{tot}} - 2.226 \text{ MeV} - E_p$. The right plot shows the same cross sections as a function of the partial wave L_p of the outgoing proton. We see strong even-odd staggering in the cross sections that probably arises from the position of the major shells in ²⁴⁰Pu with respect to the neutron threshold. The CN production cross section, at least at this low neutron energy, is seen to be as large, or larger, than the escape (breakup) cross section (red line).

By calculating both absorption and escape cross sections for a range of negative and positive neutron energies E_n , we may calculate the probability of CN capture as $P_{\rm CN} = \sigma_{\rm CN}/(\sigma_{\rm CN} + \sigma_{\rm escape})$. The results are plotted on the left of Figure 3. The probability is of course unity below the neutron escape threshold, then drops towards 0.6 as the energy rises and escape becomes possible. These new calculations for the competition between escape (breakup) and compound nucleus formation (absorption) agree qualitatively with results for (n,γ) reaction models [10, 11].



Figure 3. Results for the reaction $d + {}^{239}Pu \rightarrow p + {}^{240}Pu$ at $E_d = 15$ MeV. The left plot shows the probability of CN formation, as a function of energy across the neutron escape threshold. The right plot shows fission probabilities for neutrons incident on ${}^{239}Pu$: the new red curve shows the Britt data divided by the CN formation probability of the left plot.

On the right side of Figure 3, we repeat the curves of Figure 1, and add in the red curve which is the fission probability extracted from Britt et al., now divided by our newly calculated capture probabilities of the left side of the plot. This red curve is much closer to the probability obtained using ENDF-evaluated fission and reaction cross sections (solid black line). There are still differences between these two curves, in part because the experiment was done at proton angle of 140°, whereas our preliminary theory calculates only the ratio of angle-integrated cross sections. We also know that rotational couplings play an important role for targets such as this, while our preliminary calculations are based only on single-channel optical scattering. Future work, already underway, will remedy these shortcomings in our theory of partial fusion.

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