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Effects of direct reaction coupling in compound reactions

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Abstract. The Hauser-Feshbach (HF) model with width fluctuation correction needs to be modified when strongly coupled direct reaction channels exist. We perform cross section calculations for compound reactions which include strongly coupled channels (direct), based on the Kawai-Kerman-McVoy (KKM) theory. In KKM the cross sections are expressed in terms of channel matrix, which is given by the coupled-channels method. Numerical calculations are given for the ^{238}U elastic scattering cross sections, and the elastic enhancement factor. It is shown that the compound elastic cross sections are affected by the direct channels when the coupling is strong.

1 Introduction

The Hauser-Feshbach (HF) model [1] with width fluctuation correction, which has been widely used to calculate nuclear reaction cross sections, needs to be modified when strongly coupled direct reaction channels exist. Historically the direct reaction has been considered incoherently in the HF calculation. The direct cross sections calculated with the coupled-channels or DWBA method are simply added to or subtracted from the HF calculation. However, such a simplified correction to the HF model has not been theoretically justified, because the direct channels may change the width fluctuation effect too. In the Kawai-Kerman-McVoy (KKM) theory [2], the direct channels are explicitly included in the reaction formula in terms of the coupled channels formalism, and it enables us to evaluate the compound reaction cross sections with the direct reactions. Although the KKM theory has never been calculated numerically, this procedure is indispensable to predict reaction cross sections for strongly deformed nuclei. In this study, we solve a coupled-channels equation for actinides, and calculate the fluctuation (compound) cross sections with the KKM model. We compare the calculated cross sections with the HF model, or the HF with width fluctuation correction to investigate the effect of direct channels in the compound reactions.

2 Compound reaction at low energies

2.1 Width fluctuation correction

Since correlations exist between the incident and outgoing waves in the elastic channel, a width fluctuation correction [3] must be included in the HF formula when the number of open channels is not so large. There are several approaches [4,5] to calculate the width fluctuation correction factor W_{ab} (the elastic enhancement factor for $a = b$) defined as

$$\sigma_{ab} = \frac{\pi}{k_a^2} \cdot \frac{T_a T_b}{\sum_c T_c} W_{ab}, \tag{1}$$

where T's are the optical model transmission coefficients. Moldauer [6] obtained an expression of W_{ab}, assuming that the distribution of resonance width is a χ^2-distribution with ν channel degree of freedom. The ν parameter was evaluated by the Monte Carlo method [4], and this technique has been used because it has a great advantage in computing.

Verbaarschot, Weidenmüller, and Zirnbauer [7] derived the fluctuation cross section by assuming that Hamiltonian matrix elements form a Gaussian orthogonal ensemble (GOE), and obtained a triple integral formula. Igarasi [8], and Hilaire, Lagrange, and Koning [9] evaluated the GOE approach numerically, and showed that Moldauer's approach gives very close results to the GOE method. The systematics of ν parameter were revised by Ernebjerg and Herman [10] to give a better agreement with GOE.

It is known that the GOE approach gives the most exact results, and so does the Moldauer method. However, we should emphasize here that those theories do not consider strongly coupled direct reactions. Engelbrecht-Weidenmüller transformation [11] diagonalizes the S-matrix to reduce the problem into a diagonal form. However approximations to the width distribution are still needed to obtain the fluctuation cross sections. In the theory of Nishioka, Weidenmüller, and Yoshida [12], the direct channels are explicitly taken into account in the triple integral. However, numerical evaluations of ref. [12] have never been performed.

2.2 KKM fluctuation (compound) cross section

A common expression of S-matrix containing many resonances is

$$S_{ab}(E) = S_{ab}^{(0)}(E) - i \sum_{\lambda} \frac{\hat{g}_{\lambda_a} \hat{g}_{\lambda_b}}{E - \mathcal{E}_\lambda}, \tag{2}$$

where $S_{ab}^{(0)}(E)$ is the back-ground term, $\hat{g}_\lambda$ is the partial width amplitude, and $\mathcal{E}_\lambda$ is the complex resonance energy. This expression is inconvenient to evaluate the compound reaction cross section, because the phases of $\hat{g}_\lambda$ are not normally so random.

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KKM [2] found an equivalent expression for the S-matrix,

$$S_{ab}(E) = \overline{S}_{ab}(E) - i\sum_{q}\frac{g_{q_a}(E)g_{q_b}(E)}{E-\mathcal{E}_q}, \tag{3}$$

where $\overline{S}_{ab}(E)$ is the optical model S-matrix element, with slowly energy-dependent partial-width amplitudes $g_q(E)$. Since the phase of $g_q(E)$ is random, the energy average of the resonance sum (second term in equation (3)) becomes zero, namely $\langle S_{ab}\rangle_I \simeq \overline{S}_{ab}$. This representation simplifies the calculation of compound cross sections, and statistical properties of this representaion were numerically studied by Dagdeviren and Kerman [13].

In the overlapping-resonance limit $\Gamma \gg D$, the compound cross section can be evaluated by calculating an energy-average of fluctuation part in the S-matrix elements

$$\begin{aligned}\langle\sigma_{ab}\rangle \propto \left\langle|S_{ab}-\overline{S}_{ab}|^2\right\rangle &= \left\langle\sum_{pq}\frac{g_{q_a}g_{q_b}g^*_{p_a}g^*_{p_b}}{(E-\mathcal{E}_q)(E-\mathcal{E}_p)}\right\rangle \\ &\simeq X_{aa}X_{bb}+X_{ab}X_{ba},\end{aligned} \tag{4}$$

where $\mathbf{X}$ is the channel matrix defined by [14]

$$X_{ab} = \sqrt{2\pi/D\Gamma}\left\langle g_{q_a}g^*_{q_b}\right\rangle. \tag{5}$$

The channel matrix can be related to the coupled-channels S-matrix, in terms of the penetration matrix $\mathbf{P}$ [15]

$$\begin{aligned}P_{ab} &= \delta_{ab} - \sum_c S_{ac}S^*_{cb} \\ &= \sum_c\left\langle\sum_{pq}\frac{g_{q_a}g_{q_c}g^*_{p_c}g^*_{p_b}}{(E-\mathcal{E}_q)(E-\mathcal{E}_p)}\right\rangle \\ &\simeq \sum_c\left(X_{ab}X_{cc}+X_{ac}X_{cb}\right),\end{aligned} \tag{6}$$

which is a hermitian. With equations (4) and (6), the fluctuation cross section is given by

$$\langle\sigma_{ab}\rangle = \frac{\pi}{k_a^2}\cdot\frac{2j_a+1}{2s_a+1}\cdot\left(X_{aa}X_{bb}+X_{ab}X_{ba}\right). \tag{7}$$

The X-matrix elements are given by solving the matrix equation

$$\mathbf{P} = \mathbf{X}\mathrm{tr}(\mathbf{X}) + \mathbf{X^2}. \tag{8}$$

Since equation (8) is a non-linear equation, we solve it by using an iterative method. In the large number of open channel limit, the HF compound elastic cross section is increased by a factor of 2 ($\Gamma \gg D$) or 3 ($\Gamma \ll D$).

2.3 Transmission coefficients for inverse channels

To compare the KKM results with the HF calculations (or Moldauer's method), we have to have a correct transmission coefficient for the inverse reactions (exit channels). The transmission coefficients T_c for the exit channels are often replaced by those connecting the compound nucleus and the ground state of residual nucleus, instead of connecting the actual excited state c' to the residual nucleus

$$T_{c'}(E_{out}) \simeq T_c(E_{in}-E_x), \tag{9}$$

where E_{in} and E_{out} is the particle incident / out-going energies, and E_x is the excitation energy of the level c'. This approximation introduces further differences in the calculated results with and without direct channels.

Since the S-matrix in the coupled-channels formalism has a symmetric property, the transmission coefficients for all channels are automatically generated without the approximation of equation (9),

$$T_c = \sum_{J\Pi}\frac{2J+1}{(2I_c+1)(2j_c+1)}\left\{1-\sum_{c'}\left|S^{J\Pi}_{cc'}\right|^2\right\}, \tag{10}$$

where J and Π are the total spin and parity, I_c is the spin of the state, and the channel index c stands for either the ground state or the excited states. We evaluate T_c as in equation (10), so that the HF cross sections in this study are calculated based on a precise detailed balance.

2.4 Model parameters

Coupled-channels calculations are carried out for the neutron scattering reactions on ^{238}U. Five levels of the ground state rotational band (0^+-2^+-4^+-6^+-8^+) are coupled, and the deformed optical potential of Soukhovitskiĭ et al. [16] is employed. In this study, we exclude all the uncoupled channels, such as radiative capture and fission.

For the Moldauer calculations, three different parametrizations for the ν parameter are considered: $\nu = 1$, which corresponds to the Porter-Thomas distribution, Moldauer's systematics [4], and Ernebjerg and Herman [10].

3 Results and discussion

3.1 Compound elastic enhancement

The calculated compound elastic scattering cross section is shown in figure 1. Below the threshold energy of the first 2^+ state (44.9 keV), only the compound elastic channel is open, and all the expressions are reduced to the HF formula (namely, $\sigma_{\mathrm{CE}} = \sigma_{\mathrm{R}}^{OM}$, where σ_{R}^{OM} is the optical model compound formation cross section). Above the first excited state energy, the KKM and Moldauer theories enhance the HF cross section since it is known that the elastic enhancement factor W is greater than unity, and the KKM model gives very similar cross sections to those of Moldauer at the energies near the threshold.

The compound elastic enhancement factor W is shown in figure 2, which is defined as $\sigma/\sigma_{\mathrm{HF}}$. Note that this differs from equation (1), since W_{aa} is defined for each channel. The enhancement factors of Moldauer increase monotonously as the incident neutron energy increases, so does the number of open channels. The KKM gives the same results as Moldauer at low energies, which was already seen in figure 1, and it

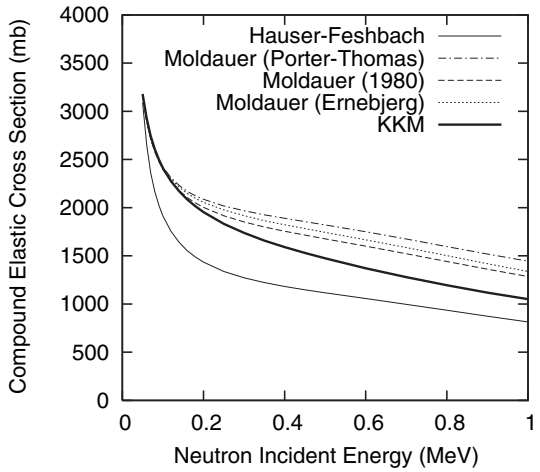

Fig. 1. Calculated compound elastic scattering cross section for ^{238}U. The thin solid line is the HF result, the KKM result is shown by the thick solid line. The Moldauer calculations are shown by the dot-dashed line ($\nu = 1$), the dashed line (ref. [4]), and the dotted line (ref. [10]).

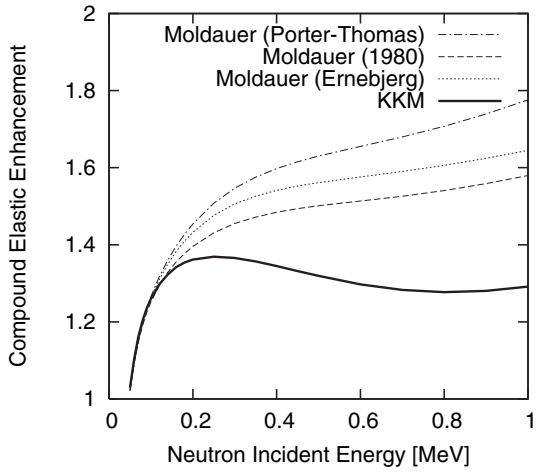

Fig. 2. Calculated compound elastic enhancement factors. The thick solid line is the KKM result, and the other lines are for the Moldauer calculations.

deviates at higher energies. This change is thought to be the direct reaction effect in the compound reaction.

Because our coupled-channels calculation does not include the excited states above 518 keV, the tendency above 680 keV might be different when those levels are included as uncoupled states. When many channels are involved, the enhancement factor rises much faster than in our calculations, and it approaches to a factor of 2, which was estimated by KKM [2], Satchler [15], and Moldauer [17].

It is understood that W decreases in the KKM case because the resonance partial-width amplitudes are affected by the direct channels coupling through the relation in equation (5), which results in changes in the compound cross sections. Moldauer's theory does not consider this effect, and the χ^2 distribution is assumed for the width distribution without the direct channels coupling.

The enhancement of elastic scattering results in decrease in the inelastic channels, because the total reaction cross section ($\sigma_{\rm R}^{OM}$) remains the same. Although the difference between KKM and Moldauer is seen in the inelastic channels too, the effect is not large.

3.2 Effect of nuclear deformation

Figure 3 shows the calculated W for the different nuclear deformation parameters β_2. In this figure, Moldauer's Monte Carlo results in ref. [4] are presented, and β_4 is set to zero. In the case of $\beta_2 = 0$ (spherical nucleus) shown by the solid curves, the tendencies of both KKM and Moldauer are very similar, and the difference is about 7% in this energy range. This difference comes from approximations made by both theories.

In the $\beta_2 = 0.3$ case, the effect of direct reaction becomes larger. The W factor of Moldauer still shows the same shape but its magnitude is changed slightly. We found that this tendency is the same for many different β_2 values. On the other hand, the direct coupling strength has a large influence on W when KKM is used. The difference between KKM and Moldauer in this case is about 20%.

In the Moldauer's method, the nuclear deformation effect comes from T_c only, which is given by the coupled-channels calculation. This is why β_2 looks insensitive to W. Since KKM explicitly includes the direct channels, the deformation effect becomes more realistic. Figure 4 shows the W factor as a function of β_2 at the neutron incident energies of 100 and 600 keV. At 100 keV KKM results (the solid curves) are very sensitive to the nuclear deformation. At this energy, the calculated compound elastic scattering cross section is 2.4 b, which is only 20% of the total elastic cross section; the shape elastic scattering is 9.2 b. Therefore, 20% difference in W becomes only 4% effect on the total elastic cross section. Even we see a large impact of the direct channels on the elastic enhancement factor, it would be difficult to confirm

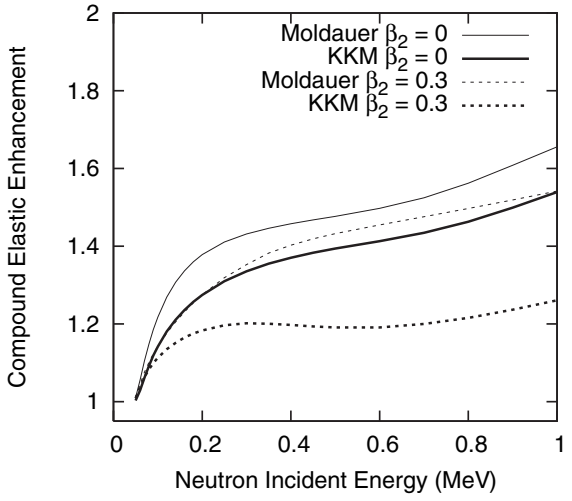

Fig. 3. Compound elastic enhancement factors for the spherical and strongly deformed cases. The thick lines are the KKM results, and the thin lines are for the Moldauer calculations.

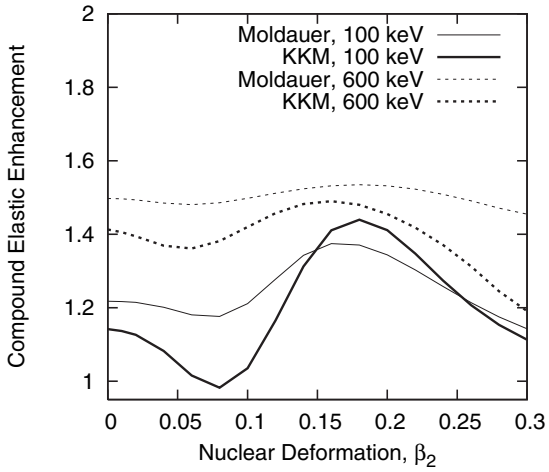

Fig. 4. Compound elastic enhancement factors as a function of β_2. The thick lines are the KKM results, and the thin lines are for the Moldauer calculations.

this effect experimentally. It means that the compound nuclear reaction calculations for deformed nuclei must be performed in a theoretically justifiable manner, with reliable nuclear deformation parameters. This would be especially important for calculating nuclear reaction cross sections of actinides for which experimental data are scarce.

4 Conclusion

We performed cross section calculations for compound reactions which include strongly coupled channels (direct), based on the Kawai-Kerman-McVoy theory [2]. Numerical calculations were given for the ^{238}U elastic scattering cross sections, and the elastic enhancement factor. The calculated results were compared with the Moldauer's theory with three different assumptions for the ν parameter. When a few channels are open and the direct coupling is not so strong, KKM and Moldauer give very similar cross sections. When strongly coupled channels exist, we found that the compound cross sections are largely affected by the direct channels. Therefore the direct channels should be included explicitly in the calculation of compound nuclear reactions.

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