Development of the Multistep Compound Process Calculation Code

Toshihiko KAWANO
Energy Conversion Engineering, Kyushu University
6-1 Kasuga-kouen, Kasuga 816, Japan
e-mail: kawano@ence.kyushu-u.ac.jp

A program "cmc" has been developed to calculate the multistep compound (MSC) process by Feshbach-Kerman-Koonin. A radial overlap integral in the transition matrix element is calculated microscopically, and comparisons are made for neutron induced ^{93}Nb reactions. Strengths of the two-body interaction V_0 are estimated from the total MSC cross sections.

1. Introduction

The quantum-mechanical theory of the pre-equilibrium nuclear reaction by Feshbach, Kerman, and Koonin[1] (FKK) has a rather simple and feasible formulation, and it has been applied to analyses of medium and high energy nuclear reactions. The theory distinguishes two types of the pre-equilibrium emission — the multistep direct (MSD) and the multistep compound (MSC).

To calculate the MSC process, the original FKK assumes constant wave functions within a nucleus because it has a great advantage to evaluate a transition matrix element easily. Milan university group[2] adopted more realistic wave functions for a bound and an unbound states, and they have developed a MSC code GAMME[3] which calculates the transition matrix elements microscopically. However open questions still exist. The calculated MSC cross section depends on an assumption of the single-particle bound states, normalization of the unbound wave functions, and a limited number of partial waves[4].

A program "cmc" was designed to show the difference between the calculations with the constant wave assumption and without it. It calculates the transition matrix element microscopically too. The bound state wave function is calculated with a harmonic oscillator or a Woods-Saxon potential, and quantum numbers of the single particle states are determined according to the shell model. The unbound state wave function is a distorted wave by a spherical optical potential.

2. The Overlap Integral

The MSC energy spectrum is given by[1]

$$\frac{d\sigma}{dU} = \frac{\pi}{k^2}\sum_J (2J+1)2\pi\frac{\langle\,,\,{}_{1J}\rangle}{\langle D_{1J}\rangle}\sum_{N=1}^{\infty}\sum_{\nu j}\frac{\langle\,,\,{}^{\uparrow\nu j}_{NJ}\rho^{\nu}(U)\rangle}{\langle\,,\,{}_{NJ}\rangle}\prod_{M=1}^{N-1}\frac{\langle\,,\,{}^{\downarrow}_{MJ}\rangle}{\langle\,,\,{}_{MJ}\rangle}, \tag{1}$$

where N is the class of the pre-equilibrium states, j is the angular momentum of the emitted particle, $2\pi\langle\,,\,{}_{1J}\rangle/\langle D_{1J}\rangle$ is the entrance strength for producing bound $2p$-$1h$ states of spin J, $\langle\,,\,{}^{\uparrow\nu j}_{NJ}\rho^{\nu}(U)\rangle$ is the escape width, $\langle\,,\,{}^{\downarrow}_{MJ}\rangle$ is the damping width, and $\langle\,,\,{}_{NJ}\rangle$ is the total width. The

escape and the damping widths are factorized by X and Y functions, $\langle , {}_{NJ}\rangle = X_{NJ}Y_N(E)$, where the Y function contains possible phase space for the transition, and the X function contains the possible angular momentum coupling and a radial overlap integral $I(j_1, j_2, j_3, j)$ between initial and final states of interaction. The overlap integral with a zero-range interaction is defined as

$$I(j_1, j_2, j_3, j) = \frac{4}{3}\pi r_0^3 V_0 \frac{1}{4\pi}\int_0^\infty u_{j_1}(r)u_{j_2}(r)u_{j_3}(r)u_j(r)\frac{dr}{r^2}, \tag{2}$$

where $u_{j_1}(r)$ and $u_{j_2}(r)$ are the single particle radial wave functions for the initial states, $u_{j_3}(r)$ and $u_j(r)$ for the final states, r_0 the radius parameter taken to be 1.2 fm, V_0 the strength of residual interaction.

When a Yukawa type residual interaction is taken into account[5], the overlap integral is given by

$$I(j_1, j_2, j_3, j) = V_0\int_0^\infty\int_0^\infty u_{j_1}(r)u_{j_2}(r)g_L(r, r')u_{j_3}(r')u_j(r')\frac{dr'}{r'^2}\frac{dr}{r^2}, \tag{3}$$

where g_L is calculated from the modified Bessel functions[6],

$$g_L(r, r') = \begin{cases} (\mu r\mu r')^{-1/2}K_{L+\frac{1}{2}}(\mu r)I_{L+\frac{1}{2}}(\mu r') & (r \geq r') \\ (\mu r\mu r')^{-1/2}I_{L+\frac{1}{2}}(\mu r)K_{L+\frac{1}{2}}(\mu r') & (r < r') \end{cases}, \tag{4}$$

where μ^{-1} is the range of interaction.

According to the assumption made by the FKK, the radial wave functions for the bound and the unbound states are constant within the nuclear volume, so that

$$u_B(r) = \sqrt{\frac{3}{R^3}}r, \qquad (r < R) \tag{5}$$

and

$$u_j(r) = \frac{4\pi}{(2\pi)^{3/2}}\frac{\sqrt{\mu kT_j}}{\hbar}r, \tag{6}$$

where $R = r_0A^{1/3}$, μ is the reduced mass, k is the wave number of the emitted particle, and T_j is the transmission coefficient. The unbound wave function carries the single particle state density of free particles inside the nuclear volume $\mathcal{V} = 4\pi R^3/3$,

$$\int_0^R |u_j(r)|^2 dr = \frac{4\pi}{(2\pi)^3}\mathcal{V}\frac{\mu k}{\hbar^2}T_j \equiv \rho_c(E_c)T_j. \tag{7}$$

To calculate the overlap integral with realistic wave functions, the unbound wave function is replaced by a distorted wave[7] normalized in unit energy,

$$\chi_j(r) = \frac{4\pi}{(2\pi)^{3/2}}\frac{\sqrt{\mu k}}{\hbar}\frac{i}{2k}\left\{H_j^*(r) - S_jH_j(r)\right\}\exp i\delta_\ell, \tag{8}$$

where $H_j(r) = G_j(r) + iF_j(r)$ is the outgoing-wave Coulomb function, S_j the scattering matrix element, and δ_ℓ the Coulomb phase shift.

The bound wave function is calculated with a harmonic oscillator or a Woods-Saxon potential. The quantum numbers and the binding energies of the bound states are determined according to the spherical Nilsson model. These wave functions for $\ell = 0$, 1, 2 and 3, are shown in Fig.1. They are the radial wave functions of $2s_{1/2}$, $1p_{1/2}$, $0d_{5/2}$, and $1f_{7/2}$ states in the Woods-Saxon potential of $V = 50$ MeV, $V_{so} = 7$ MeV, $r = 1.2$ fm, and $a = 0.7$ fm, and the harmonic oscillator with $\hbar\omega = 41A^{-1/3}$. Usually there are several configurations for a possible transition for a given angular momentum transfer. For example, both $I(s_{1/2}, p_{1/2}, d_{5/2}, f_{7/2})$

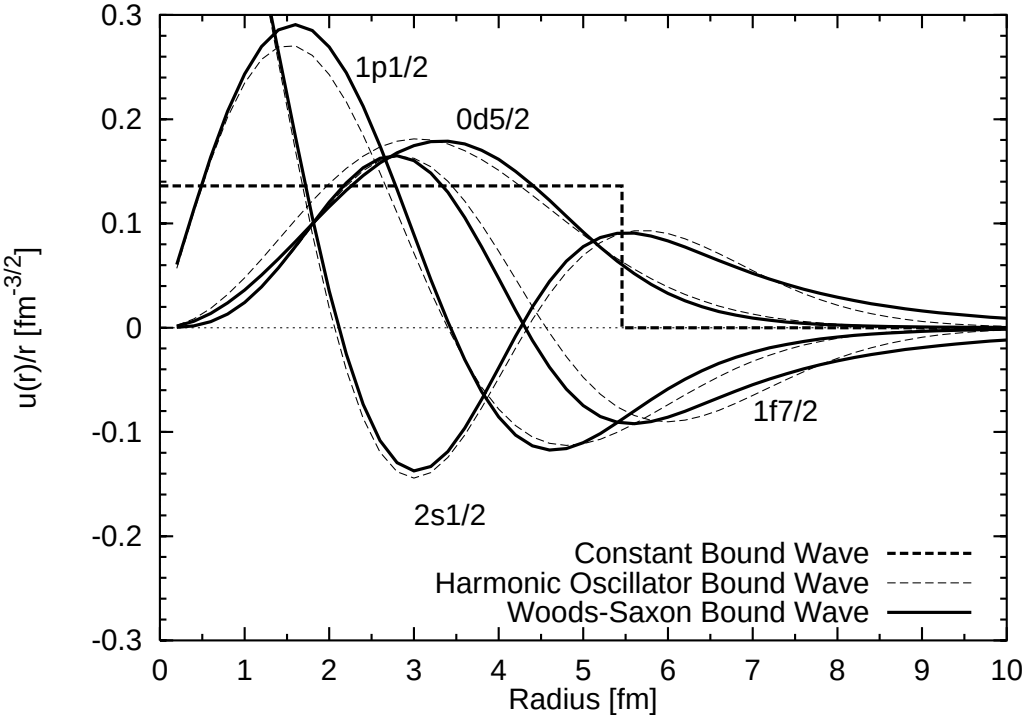

Fig.1: Comparison of the shell model wave functions and the constant wave

and $I(s_{1/2}, p_{1/2}, d_{3/2}, f_{7/2})$ are possible for the case above. These overlap integrals are averaged to give an appropriately averaged matrix element.

The overlap integrals for this configuration are, $I_B/V_0 = 0.0106$ for the constant wave, 3.38×10^{-5} for the harmonic oscillator, and 1.21×10^{-5} for the Woods-Saxon potential. These values strongly depend on a choice of the interacting particles and holes, but the averaged values over various configurations are almost independent. The averaged overlap integrals are, $\bar{I_B}/V_0 = 5.80 \times 10^{-3}$ for the harmonic oscillator, and 7.07×10^{-3} for the Woods-Saxon.

The constant wave function approximation generally overestimates the overlap integrals of not only a bound/bound configuration but also a bound/unbound configuration. This overestimate cancels in the ratio of the widths $\langle , {}^{\uparrow\nu j}_{NJ}\rho^{\nu}(U)\rangle$ and $\langle , {}^{\downarrow}_{MJ}\rangle$ to the total width $\langle , {}_{NJ}\rangle$, and one obtains simple estimates for the ratio regardless of details of the interaction[8]. The approximation has an advantage for the calculation of a composite system decay rate because it contains the ratio only, however it is invalid if one calculates the entrance strength microscopically because it is proportional to the width of the $2p$-$1h$ doorway state.

3. The Entrance Strength Function

From Eq.(1), the emission and the damping probabilities can be calculated regardless to the two-body residual interaction V_0, since V_0 cancels in the ratio of the emission and damping widths to the total width. The entrance strength still holds V_0 and one can estimate the strength of V_0 if the entrance strength is calculated microscopically[9],

$$2\pi \frac{\langle , {}_{1J}\rangle}{\langle D_{1J}\rangle} = (2\pi)^2 \omega(2,1,E) \sum_{Q j_3} (2Q+1)(2j_3+1) F(Q) R_1(j_3) \begin{pmatrix} j & j_3 & Q \\ 0 & 0 & 0 \end{pmatrix}^2 I^2(j_1, j_2, j_3, j), \quad (9)$$

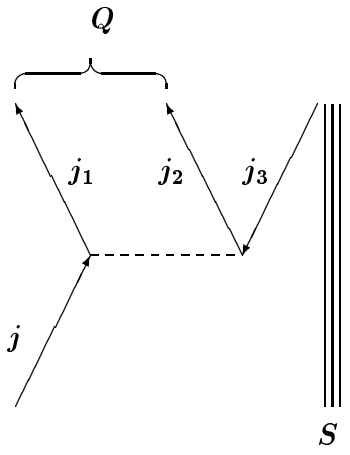

Fig.2: The angular momentum coupling scheme for the entrance channel. The incident particle j is captured in the single particle orbit j_1, creating the particle-hole pair j_2 and j_3

where the angular momentum coupling scheme is defined in Fig.2, $\omega(2,1,E)$ is the $2p$-$1h$ state density at the excitation energy E, and $F(Q)$ is the angular momentum density:

$$F(Q) = \sum_{j_1} \sum_{j_2} (2j_1+1)(2j_2+1) R_1(j_1) R_2(j_2) \begin{pmatrix} j_1 & j_2 & Q \\ 0 & 0 & 0 \end{pmatrix}^2, \tag{10}$$

where $R(j)$ is the spin distribution of the state.

Chadwick and Young[10] found that the entrance strength can be evaluated by the optical model transmission coefficients corrected by a factor $R^{\rm MSC} = \omega^B(2,1,E)/\omega(2,1,E)$, which is the fraction of flux into the bound $2p$-$1h$ state. The entrance strength becomes

$$2\pi \frac{\langle , {}_{1J}\rangle}{\langle D_{1J}\rangle} = R^{\rm MSC} T_J. \tag{11}$$

Figure 3 shows the calculated strengths for 14 MeV neutron-induced ^{93}Nb reactions (multiplied by $(2J+1)\pi/k^2$ to give an initial $2p$-$1h$ state formation cross section). The distorted wave and the transmission coefficient are calculated with the Walter-Guss' global optical potential[11]. The single-particle state density parameter g is taken as $g = A/13$ MeV^{-1}, and the pairing energy correction $\Delta = 0$. The solid line is calculated according to the coupling scheme in Fig.2, and the total reaction cross section is normalized to the value given by Eq.(11). At the microscopic calculation, the particle and the hole states which obey angular momentum and energy conservation are included. It restricts the possible final states, and results in small cross sections for large J.

The initial $2p$-$1h$ state formation cross section is proportional to V_0^2 when Eq.(9) is employed, and it is possible to estimate V_0 roughly if one compares the cross sections given by Eq.(9) and those by Eq.(11). Figure 4 shows the $2p$-$1h$ state formation cross sections for neutron-induced ^{93}Nb reactions as functions of the incident energy. The solid line is calculated from Eq.(9) with $V_0 = 10.4$ MeV, and the dotted line is Eq.(11). The value of V_0 was chosen to give the same cross section at 14 MeV, and it is larger than the value of 5 MeV obtained by Bonetti, *et al.*[4].

If one assumes the constant wave for the entrance strength calculation[12], it yields large overlap integrals as indicated in the previous section, and results in small V_0. Only 450 keV of V_0 gives the same strength at 14 MeV.

The $2p$-$1h$ formation cross section with the range of 1 fm is shown in Fig.4 by the dashed line. The effect of inclusion of the finite-range correction is very large, but it can be compensated if one adjusts V_0 appropriately. The calculated cross sections are about 30% of the zero-range results, and 19 MeV of V_0 gives almost the same cross sections.

4. Conclusion

A multistep compound process calculation program "cmc" has been developed to calculate an overlap integral microscopically. An entrance strength of the initial MSC process was calculated for ^{93}Nb+n(14 MeV), and it gave a rough estimation for V_0 of about 10.4 MeV for a zero-range interaction, and 19 MeV for a Yukawa interaction with the range of 1 fm.

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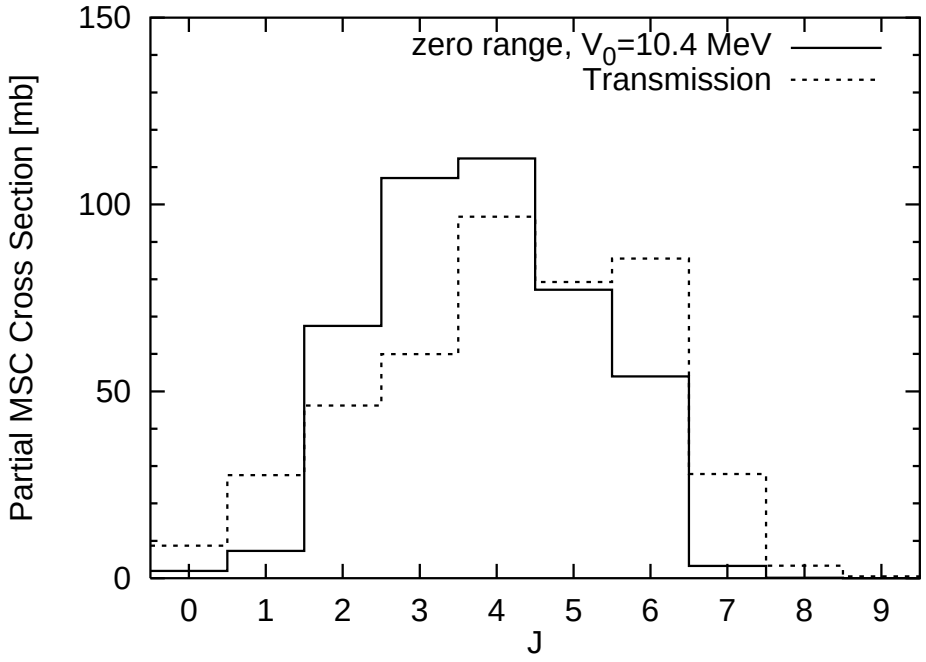

Fig.3: Comparison of the partial cross sections calculated from Eq.(9) and Eq.(11)

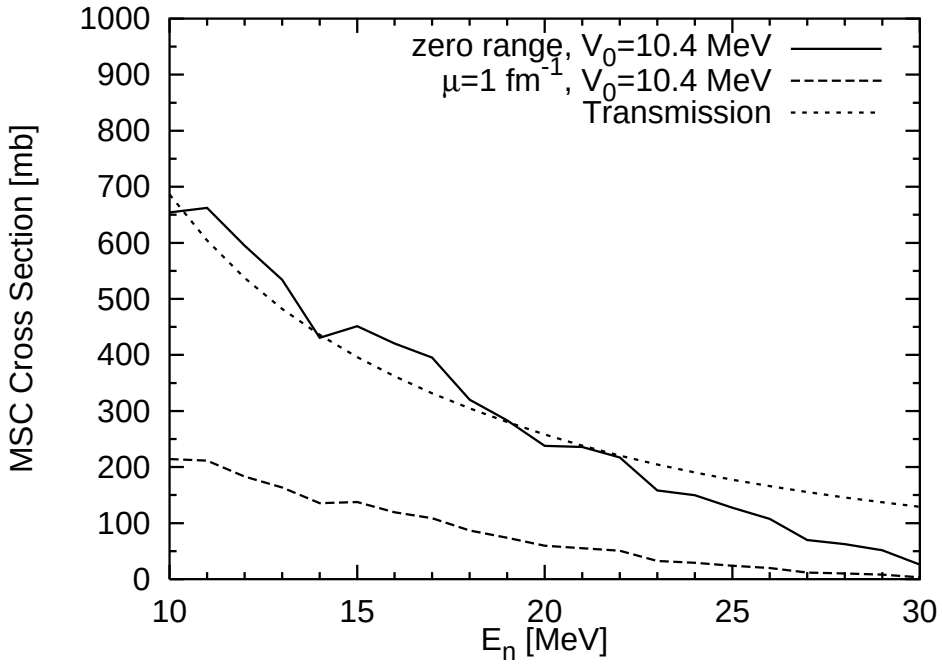

Fig.4: Comparison of the total MSC cross sections calculated from Eq.(9) and Eq.(11)