Master equation approach to statistical multistep compound reactions

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A master equation is incorporated in Feshbach, Kerman, and Koonin model calculations of statistical multistep compound (MSC) emission. Damping X and Y functions which describe the particle-hole annihilation process are derived. The MSC cross sections are calculated with the master equation. The effect is found to be large at lower energies for light nuclei, but not significant when the incident energy is above 20 MeV. The difference between a closed form solution and the master equation result is masked by the large multistep direct and evaporation components. [S0556-2813(98)02002-0]

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A *never-come-back* approximation is often made for calculations of the pre-equilibrium particle emission cross sections. The approximation is valid at high excitation energies and at early stages in the process [1], since transitions to the states of greater complexity are more probable than transitions to the states of lesser complexity, and one can neglect the transition that decreases the number of excitons.

This *never-come-back* approximation simplifies the calculation of pre-equilibrium emission, and it is adopted by the Feshbach, Kerman, and Koonin (FKK) theory [2] to evaluate the multistep compound (MSC) process. The particle-hole annihilation process is, however, important at low excitation energies and at the stages near the equilibrium state where many excitons are excited simultaneously, and one has to solve a master equation [3,4] to calculate the MSC cross section. We showed some examples of the master equation calculations briefly in Ref. [5]. Here we provide the master equation expression for the MSC cross section, and demonstrate the effect of use of the master equation.

The MSC energy spectrum with the *never-come-back* assumption is given by [2]

$$\frac{d\sigma}{d\varepsilon}=\frac{\pi}{k^2}\sum_J (2J+1) \times 2\pi\frac{\langle\Gamma_{1J}\rangle}{\langle D_{1J}\rangle}\sum_N \sum_{\nu j} \frac{\langle\Gamma_{NJ}^{\uparrow\nu j}\rho^\nu(U)\rangle}{\langle\Gamma_{NJ}\rangle}\prod_{M=1}^{N-1}\frac{\langle\Gamma_{MJ}^{\downarrow}\rangle}{\langle\Gamma_{MJ}\rangle}, \quad (1)$$

where ν labels the three exit modes ($\Delta N=0$ and ± 1), $2\pi(\langle\Gamma_{1J}\rangle/\langle D_{1J}\rangle)$ is the entrance strength for producing bound $2p$-$1h$ states of spin J. $\langle\Gamma_{NJ}^{\uparrow\nu j}\rho^\nu(U)\rangle$ is the escape width, $\langle\Gamma_{MJ}^{\downarrow}\rangle$ is the damping width, and $\langle\Gamma_{NJ}\rangle$ is the total width.

The escape and damping widths are factorized by X and Y functions, $\langle\Gamma_{NJ}\rangle=X_{NJ}Y_N(E)$. The X function contains the possible angular momentum coupling and overlap integrals between initial and final states of interaction. The Y function contains the possible phase space for the transition.

The X and Y functions for the escape process $X^{\uparrow N\pm 1}$, $X^{\uparrow N}$, $Y^{\uparrow N\pm 1}$, and $Y^{\uparrow N}$, and for the damping process $X^{\downarrow N+1}$ and $Y^{\downarrow N+1}$ in which the number of excitons changes by $+2$, are defined by FKK in Ref. [2]. More practical and simple formulations are shown in Refs. [6] and [7]. In order to calculate the particle-hole pair annihilation process we have to define the X and Y functions for the damping process in which the number of excitons decreases.

The damping X function can be obtained from the $X^{\uparrow N-1}$ function multiplied by the final spin state density $R_1(j)$, summing it over j,

$$X_{NJ}^{\downarrow N-1}=2\pi\sum_{SjQj_3}(2j_3+1)(2Q+1) \times\frac{R_{n-3}(S)R_1(j_3)R_1(j)}{R_n(J)}F(Q) \times\begin{pmatrix} j & j_3 & Q\\ 0 & 0 & 0\end{pmatrix}^2 I^2(j_1,j_2,j_3,j)\Delta(jSJ), \quad (2)$$

where $\Delta(jSJ)$ is the triangle function, $I(j_1,j_2,j_3,j)$ the overlap integral, and $R_n(j)$ the Gaussian angular momentum distribution with spin cutoff $\sigma^2=0.24nA^{2/3}$ [8]. The diagram of the angular momenta in Eq. (2) is shown in Fig. 1.

Two processes contribute to the $Y^{\downarrow N-1}$. One is the scattering of a bound nucleon annihilating the particle-hole pair given by

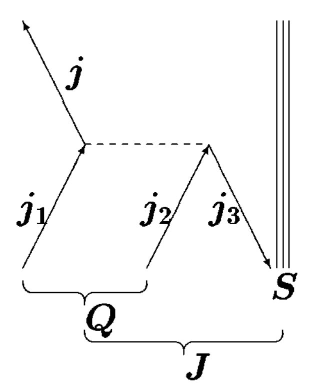

FIG. 1. The X function for the $\Delta n=-2$ process.

$$
\begin{aligned}
{}_{a}Y_{N}^{\downarrow N-1}(E) &= \int_{z} \frac{\omega(p-2,h-1,z)}{\omega(p,h,E)}\,\omega(2,1,E-z)\,\omega(1,0,E-z)\,dz \\
&= \frac{1}{2}\,\frac{g_c^4}{\omega(p,h,E)}\left\{ \frac{\omega(p-2,h-1,E^{n-1}) - \omega(p-2,h-1,(E-B)^{n-1})}{(n-3)(n-2)(n-1)} \right. \\
&\qquad \left. - \frac{B\,\omega(p-2,h-1,(E-B)^{n-2})}{(n-3)(n-2)} - \frac{B^2\omega(p-2,h-1,(E-B)^{n-3})}{2(n-3)} \right\}, \qquad (3)
\end{aligned}
$$

and the other is the hole scattering,

$$
\begin{aligned}
{}_{b}Y_{N}^{\downarrow N-1}(E) &= \int_{z} \frac{\omega(p-1,h-2,z)}{\omega(p,h,E)}\,\omega(1,2,E-z)\,\omega(0,1,E-z)\,dz \\
&= \frac{1}{2}\,\frac{g_c^4}{\omega(p,h,E)}\left\{ \frac{\omega(p-1,h-2,E^{n-1}) - \omega(p-1,h-2,(E-B)^{n-1})}{(n-3)(n-2)(n-1)} \right\}, \qquad (4)
\end{aligned}
$$

where $\omega(p,h,E)$ is the density of a p-particle h-hole configuration at an excitation energy E, with the nucleons restricted to energies below the binding energy B, g_c is the single-particle state density parameter of the composite system. These two processes are shown in Fig. 2. The total damping $Y^{\downarrow N-1}$ function is a sum of these Y functions.

With Eqs. (2), (3), and (4), the energy spectrum for the MSC process including the particle-hole annihilation can be calculated by

$$
\frac{d\sigma}{d\varepsilon} = \frac{\pi}{k^2}\sum_{J}(2J+1) \times 2\pi\frac{\langle\Gamma_{1J}\rangle}{\langle D_{1J}\rangle}\sum_{N}\sum_{\nu j}\langle\Gamma_{NJ}^{\uparrow\nu j}\rho^{\nu}(U)\rangle\int_0^{t_{eq}}P_J(N,t)\,dt, \qquad (5)
$$

where t_{eq} is the equilibration time, and $P_J(N,t)$ is the time-dependent occupation probability which satisfies the following master equation:

$$
\begin{aligned}
\frac{dP_J(N,t)}{dt} &= P_J(N-1,t)\langle\Gamma_{N-1\,J}^{\downarrow N+1}\rangle + P_J(N+1,t)\langle\Gamma_{N+1\,J}^{\downarrow N-1}\rangle \\
&\quad - P_J(N,t)\left\{\langle\Gamma_{NJ}^{\downarrow N+1}\rangle + \langle\Gamma_{NJ}^{\downarrow N-1}\rangle \right. \\
&\quad \left. + \sum_{\nu j}\int\langle\Gamma_{NJ}^{\uparrow\nu j}\rho^{\nu}(U)\rangle dU\right\}. \qquad (6)
\end{aligned}
$$

Neglecting $\langle\Gamma^{\downarrow N-1}\rangle$ in Eq. (6) leads to the closed form expression which is equivalent to the original FKK.

The entrance strength in Eqs. (1) and (5) can be evaluated by the optical model transmission coefficients corrected by a factor R^{MSC}, which is the fraction of flux into the bound $2p$-$1h$ state, as in Ref. [7].

The overlap integral I in the X functions contains the wave functions of bound single-particle states. We use the constant wave functions for the bound-unbound and bound-bound overlap integrals. This assumption is rather artificial, but it has the great advantage of calculating the overlap integral easily. The simplification was made by Chadwick and Young [7] and they showed that the calculated results are in good agreement with the experimental data.

In Fig. 3 we present the damping Y functions for the $\Delta N = \pm 1$ process in the neutron induced reactions on ^{93}Nb. The single-particle state density parameter g is taken as $g = A/13\ \mathrm{MeV}^{-1}$, and the pairing energy correction $\Delta = 0$. The $Y_N^{\downarrow N-1}$ functions increase rapidly with increase in complexity of the states, and at the $N=8$ stage it is more probable to annihilate the particle-hole pairs. At this stage MSC chaining should be terminated because an occupation probability of more complicated configurations becomes small, and subsequent interactions lead to a full equilibrium stage which yields an evaporation spectrum.

The master equation in Eq. (6) is solved numerically [3]. Figure 4 shows a result of the master equation calculation for ^{93}Nb(n,n') at $E_n = 14$ MeV and $J=0$, which is the time evolution of the occupation probabilities. The Walter-Guss optical potential parameters [9] are used for neutrons and protons. The shape of the occupation probability distribution converges as time increases, and the equilibration time t_{eq} in Eq. (5) is determined by the condition

$$
\frac{P_J(N,t-\delta t)/\Sigma_N P_J(N,t-\delta t)}{P_J(N,t)/\Sigma_N P_J(N,t)} < 10^{-5}. \qquad (7)
$$

Comparisons of the master equation and closed form calculations for ^{93}Nb(n,n') and (n,p) at $E_n = 14$ MeV are

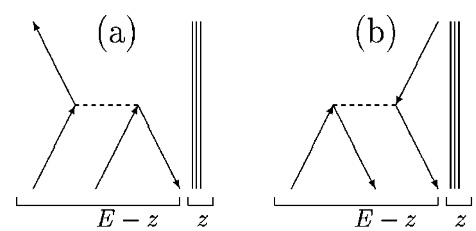

FIG. 2. The two damping processes, corresponding to a particle or a hole scattering with the bound nucleon, annihilating a particle-hole pair. The energy of the interacting particles is $E-z$, where z is the core energy and E is the initial total energy.

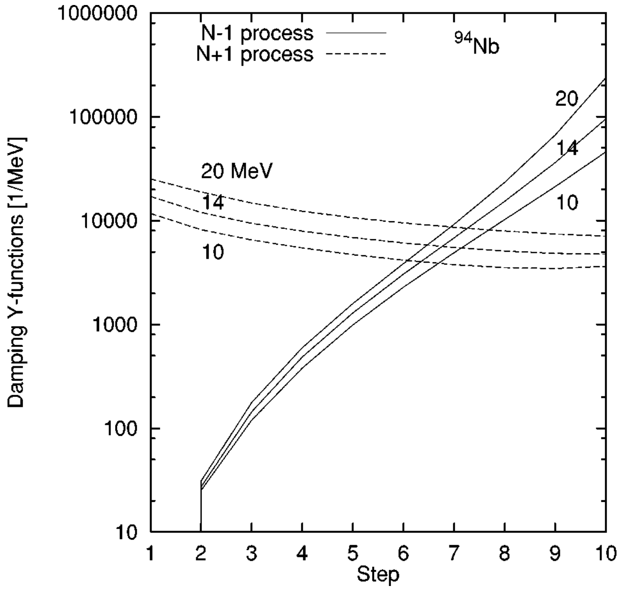

FIG. 3. The ^{94}Nb damping Y functions for incident neutron energies of 10, 14, and 20 MeV. The solid lines are the $\Delta N=-1$ process, and the dashed lines are the $\Delta N=+1$ process.

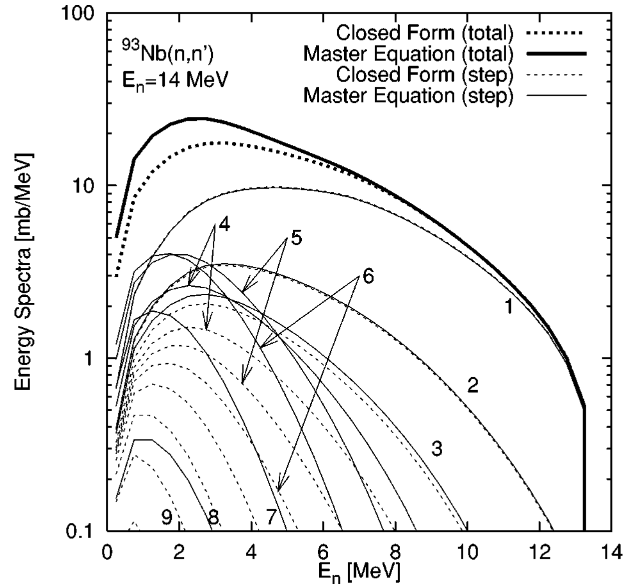

FIG. 5. Comparison of the master equation and closed form calculations for ^{93}Nb(n,n') at $E_n=14$ MeV. The solid lines are the master equation calculation, the dotted lines are the closed form calculation, and the heavy lines are the total MSC spectra.

shown in Figs. 5 and 6, respectively. The master equation calculation enhances particle emissions from $N\geqslant 4$ stages. The effect is large for the low energy neutron emission process. At the stages of $N\leqslant 3$, the differences between the master equation and the closed form results are very small. The total MSC spectrum by the master equation becomes softer than that by the closed form calculation. For (n,p) reactions, particle emissions from $N\geqslant 4$ stages are less important relative to the leading three stages because of the Coulomb barrier, thus the effect of the master equation calculation is small as seen in Fig. 6.

Calculated MSC spectra for ^{93}Nb(n,n') at $E_n=25$ MeV are shown in Fig. 7. The difference between the closed form and the master equation calculations becomes small as the incident energy increases. At 14 MeV, 26.3% of the formation cross section for the initial $2p$-$1h$ state is emitted from the leading two stages. This fraction increases with the incident energy, and it rises up to 77.1% at 25 MeV. Thus the relative importance of the $N\geqslant 3$ stages decreases, and the master equation calculation becomes insensitive to the total MSC cross section.

Ratios of the total MSC cross sections calculated with the master equation to those with the closed form expression for (n,n') and (n,p) reactions on ^{27}Al, ^{56}Fe, and ^{93}Nb are shown in Fig. 8. The effect of using the master equation is large for light nuclei at low incident energies. The neutron emission from medium nuclei at 14 MeV is enhanced to about 40%. However, the observed particle emission cross

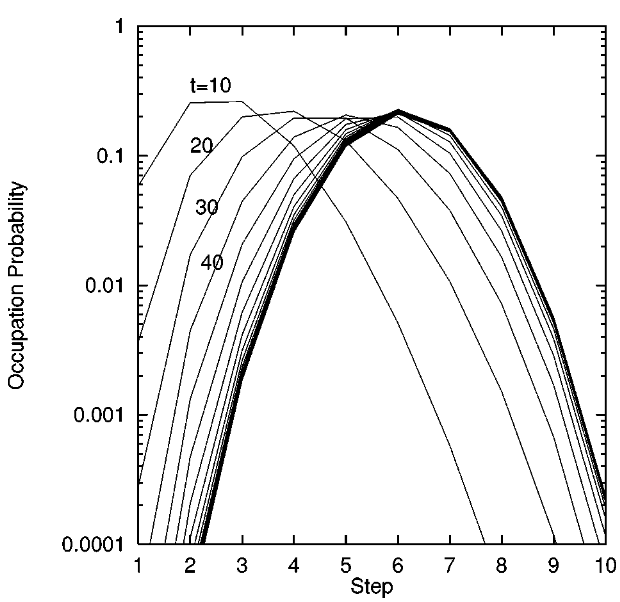

FIG. 4. The result of the master equation calculation. The occupation probability $P_J(N,t)$ for ^{93}Nb(n,n') at $E_n=14$ MeV, $J=0$. The time has a unit of $\hbar/2\pi$.

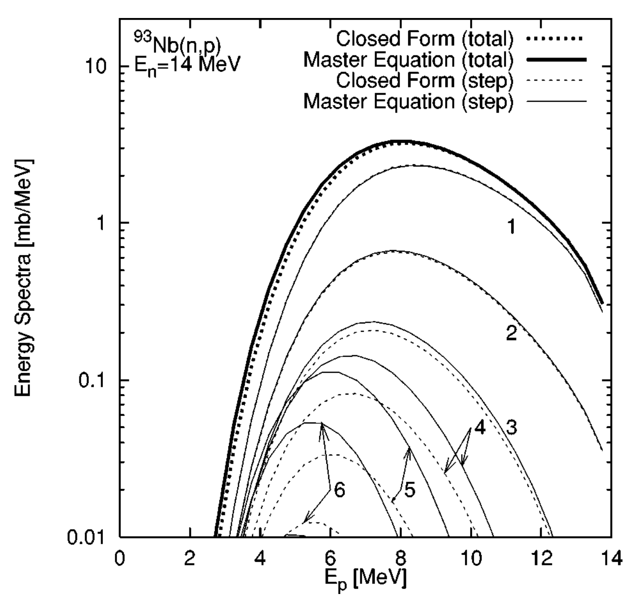

FIG. 6. Same as Fig. 5 but ^{93}Nb(n,p) at $E_n=14$ MeV.

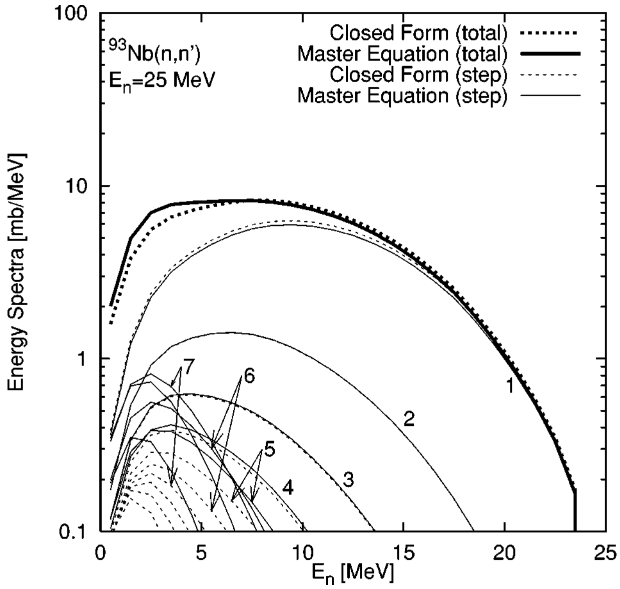

FIG. 7. Same as Fig. 5 but ^{93}Nb(n,n') at $E_n = 25$ MeV.

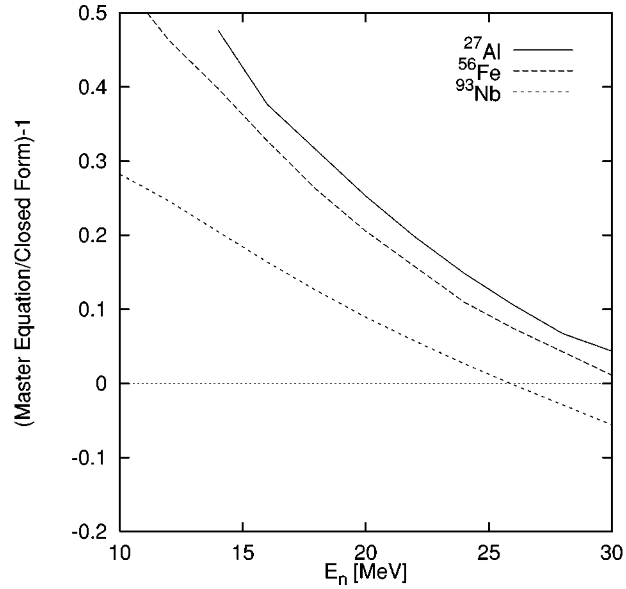

FIG. 8. Ratio of the total MSC cross sections calculated with the master equation to those with the closed form for (n,n') and (n,p) reactions on ^{27}Al, ^{56}Fe, and ^{93}Nb. The ratio is expressed by $\sigma_{\text{master}}/\sigma_{\text{closed}} - 1$ where σ_{master} and σ_{closed} are the total MSC cross sections.

sections at these energies comprise MSD, MSC, and evaporation components. A larger MSC emission from the master equation approach results in a smaller evaporation component, and the difference in the total emission spectra between the master equation and the closed form becomes smaller. At energies above 20 MeV where the MSD contribution dominates, the master equation effect in the MSC is expected to be masked by the large MSD and evaporation components.

In conclusion, we have derived a master equation expression for the FKK MSC process. The calculated MSC cross section shows that the effect of the master equation is large for light nuclei at low energies. It is, however, negligible above 20 MeV.

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