RAPID COMMUNICATIONS

PHYSICAL REVIEW C VOLUME 51, NUMBER 3 MARCH 1995

Linking of direct and compound chains in multistep nuclear reactions

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(Received 12 October 1994)

We remove the sharp separation between multistep compound and multistep direct emission in the Feshbach-Kerman-Koonin (FKK) derivation of preequilibrium processes. In addition to the original multistep compound mechanism, we find a new class of multistep processes arising from linking of the direct and compound chains. There can be additional scatterings in unbound P space before the quasibound compound Q space is entered, or after it is left. We provide a theoretical justification for the presence of $P \rightarrow Q$ transitions, which are needed to account for experimentally observed preequilibrium spectra. Our formalism is applied to the analysis of the 14 MeV ^{93}Nb(n,n') reaction, using modified distorted-wave Born approximation (DWBA) matrix elements which include an inverse S-matrix factor. Since the dominant contribution to multistep compound emission comes from the *2p1h* Q stage, the linking of the multistep chains results in flux bypassing this stage, resulting in a reduced multistep compound emission and an increased emission from the compound nucleus.

PACS number(s): 24.60.Gv, 24.60.Dr, 25.40.Fq, 24.50.+g

The multistep theory of nuclear reactions presented by Feshbach, Kerman, and Koonin (FKK) in Ref. [1] has been applied to a wide variety of neutron- and proton-induced reactions for incident energies up to 250 MeV. For reviews see Refs. [2,3]. FKK showed that the quantum statistics of multistep processes involving quasibound and unbound particle-hole states differ, and separated preequilibrium processes into two categories: multistep compound (MSC), which occurs when a chain of quasibound (Q) states is excited, and multistep direct (MSD), which occurs when a chain of states always involving at least one unbound particle (P) is excited. This sharp separation into bound and unbound chains seemed somewhat artificial, and resulted in some criticisms of the theory, even though other quantum theories of multistep processes published after FKK also relied on this distinction. However, Nishioka, Weidenmüller, and Yoshida [4] considered the influence of MSD on transmission coefficients into the Q chain in their multistep theory. Formal expressions were given, but no calculations were performed because of numerical difficulties in computing multistep processes in their theory.

The importance of transitions from the P to Q chains was first noted in FKK analyses of the emission spectra in 14 MeV neutron-induced reactions [5]. These processes were found to be necessary in order to obtain the correct magnitude of MSC emission. Subsequently, Ref. [6] analyzed neutron reactions on niobium between 14 and 26 MeV and showed that an accurate description of experimental emission spectra and angular distributions required the inclusion of $P \rightarrow Q$ transitions. Marcinkowski *et al.* [7,8] also analyzed experimental emission spectra for a range of target nuclei in 20 MeV neutron-induced reactions, and emphasized the need for a gradual absorption into the compound chain. A number of other recent analyses of data have included these mechanisms [9,10]. All these approaches estimated the strength of crossover transitions from a phenomenological phase-space model, considering the densities of P and Q states [6–8]. While such estimates were checked against the experimentally observed partitioning of MSC and MSD and found to be rather reliable [6], there is a need to justify $P \rightarrow Q$ transitions theoretically. Following the work of Nishioka *et al.*, Sato and Yoshida [11] recently investigated the influence of the imaginary part of the optical potential on transitions into the compound chain. Their results supported the predictions based upon phase-space linking, though there were indications that it might overestimate the effect. In this paper we remove the approximation in the FKK derivation which led to the sharp separation of MSC and MSD, and we show how our new derivation naturally incorporates processes linking these two preequilibrium chains.

In the original formulation of the FKK theory the transition matrix element $\mathscr{T}_{fi}$ was decomposed into a direct and a fluctuating component:

$$\mathscr{T}_{fi}=\mathscr{T}_{fi}^{\mathrm{MSD}}+\mathscr{T}_{fi}^{\mathrm{MSC}}. \tag{1}$$

The fluctuating component is given by

$$\mathscr{T}_{fi}^{\mathrm{MSC}}=\left\langle \Psi_f^{(-)}\middle| V_{PQ}\frac{1}{E-h_{QQ}}V_{QP}\middle|\Psi_i^{(+)}\right\rangle, \tag{2}$$

where

$$h_{QQ}=H_{QQ}+V_{QP}\frac{1}{E^{(+)}-H_{\mathrm{opt}}}V_{PQ}. \tag{3}$$

Here $V_{PQ}=H_{PQ}\sqrt{iI/(E-H_{QQ}+iI)}$ [12], I is the energy averaging interval, and $\Psi_i^{(+)}$ is the distorted wave solution of H_{opt} with outgoing boundary condition. As was done in [1], H_{opt} will be separated into its diagonal and off-diagonal components $H_{\mathrm{opt}}=H_{\mathrm{opt}}^{(D)}+v$, so that

$$|\Psi_i^{(+)}\rangle=|\phi_i^{(+)}\rangle+\frac{1}{E^{(+)}-H_{\mathrm{opt}}}v|\phi_i^{(+)}\rangle, \tag{4}$$

where $(E-H_{\rm opt}^{(D)})|\phi_i^{(+)}\rangle=0$. In the FKK paper the above wave function $|\Psi_i^{(+)}\rangle$ in Eq. (2) was approximated by the first term, i.e., $|\Psi_i^{(+)}\rangle\approx|\phi_i^{(+)}\rangle$, and likewise for $\langle\Psi_f^{(-)}|$. By removing this approximation, and inserting the complete expression for the wave functions $|\Psi_i^{(+)}\rangle$ and $\langle\Psi_f^{(-)}|$ into Eq. (2), four terms are obtained,

$$\mathscr{T}_{fi}^{\rm MSC}=\mathscr{T}^{Q}+\mathscr{T}^{PQ}+\mathscr{T}^{QP}+\mathscr{T}^{PQP}, \tag{5}$$

where

$$\mathscr{T}^{Q}\equiv\left\langle\phi_f^{(-)}\left|V_{PQ}\frac{1}{E-h_{QQ}}V_{QP}\right|\phi_i^{(+)}\right\rangle, \tag{6}$$

$$\mathscr{T}^{PQ}\equiv\left\langle\phi_f^{(-)}\left|V_{PQ}\frac{1}{E-h_{QQ}}V_{QP}\frac{1}{E-H_{\rm opt}}v\right|\phi_i^{(+)}\right\rangle, \tag{7}$$

$$\mathscr{T}^{QP}\equiv\left\langle\phi_f^{(-)}v\left|\frac{1}{E-H_{\rm opt}}V_{PQ}\frac{1}{E-h_{QQ}}V_{QP}\right|\phi_i^{(+)}\right\rangle, \tag{8}$$

$$\mathscr{T}^{PQP}\equiv\left\langle\phi_f^{(-)}\left|v\frac{1}{E-H_{\rm opt}}V_{PQ}\frac{1}{E-h_{QQ}}V_{QP}\frac{1}{E-H_{\rm opt}}v\right|\phi_i^{(+)}\right\rangle. \tag{9}$$

Only the first term in Eq. (5) was analyzed in the original FKK theory (where it was denoted by $\mathscr{T}_{fi}^{\rm MSC}$ instead of $\mathscr{T}^{Q}$), and the other terms were omitted. The three extra terms describe processes where there are additional scatterings in the P chain before and/or after passing through the Q chain. They are still classed within MSC since the random phase approximation ensures that they yield angular distributions symmetric about 90° (once excitations take place in the Q chain the "memory" of the initial projectile direction is always lost). Figure 1 shows a schematic representation of the four MSC types, with definitions of our labelings of P and Q stages.

In determining the average of $\mathscr{T}_{fi}^{\rm MSC}\mathscr{T}_{fi}^{\rm MSC*}$, which is needed to obtain the cross section, we expand each of the four terms as a summation over the number of preequilibrium stages through which the excited nucleus passes before decay. For the processes originally considered by FKK, this entails summing over n, but for the new processes it brings in additional summations over the P stage from which the Q space is entered (μ) and the P stage from which emission finally occurs occurs (λ); see Fig. 1. Cross terms (e.g., $\langle\mathscr{T}^{PQ}\mathscr{T}^{Q*}\rangle$) vanish due to the random phase hypothesis, yielding

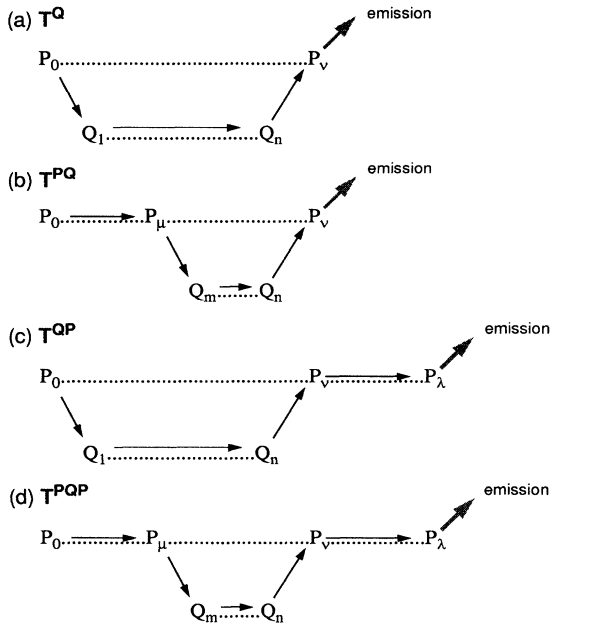

FIG. 1. Diagrammatic representation of the four MSC processes. FKK originally considered only process (a).

$$\langle|\mathscr{T}_{fi}^{\rm MSC}|^2\rangle=\sum_{n=1}^{r}\langle|\mathscr{T}_{n}^{Q}|^2\rangle+\sum_{\mu n}^{r}\langle|\mathscr{T}_{\mu n}^{PQ}|^2\rangle+\sum_{n\lambda}^{r}\langle|\mathscr{T}_{n\lambda}^{QP}|^2\rangle+\sum_{\mu n\lambda}^{r}\langle|\mathscr{T}_{\mu n\lambda}^{PQP}|^2\rangle, \tag{10}$$

where the meaning of the indices in the above equation is shown in Fig. 1, and r labels the equilibrium stage.

To illustrate, $\mathscr{T}_{\mu n\lambda}^{PQP}$ describes a process in which the projectiles undergoes MSD-type scatterings until reaching the P_μ subspace, enters the Q_m subspace (where $m=\mu,\mu\pm1$ by chaining), follows the MSC Q chain until the Q_n subspace, returns to the P_ν subspace (where $\nu=n,n\pm1$ by chaining), undergoes more MSD-type rescatterings, and is finally emitted from the P_λ subspace. Since the other transition matrix elements $\mathscr{T}_{n}^{Q}$, $\mathscr{T}_{n\lambda}^{QP}$, and $\mathscr{T}_{\mu n}^{PQ}$ can be viewed as special cases of the $\mathscr{T}_{\mu n\lambda}^{PQP}$ transition, we only evaluate this process, from which the others may be inferred:

$$\mathscr{T}_{\mu n\lambda}^{PQP}=\left\langle\phi_f^{(-)}\left|v_{P_fP_\lambda}\frac{1}{E-H_{\rm opt}}V_{P_\nu Q_n}\frac{1}{E-h_{QQ}}V_{Q_mP_\mu}\frac{1}{E-H_{\rm opt}}v_{P_1P_0}\right|\phi_i^{(+)}\right\rangle, \tag{11}$$

which, upon the FKK factorization of the Green's functions, along with the "chaining hypothesis," becomes

$$\mathscr{T}_{\mu n\lambda}^{PQP}=\langle\phi_f^{(-)}|v_{P_fP_\lambda}G_{P_\lambda}v_{P_\lambda P_{\lambda-1}}\cdots V_{P_\nu Q_n}G_{Q_n}V_{Q_nQ_{n-1}}\cdots G_{Q_m}V_{Q_mP_\mu}G_{P_\mu}\cdots G_{P_1}v_{P_1P_0}|\phi_i^{(+)}\rangle. \tag{12}$$

In deriving expressions for MSC emission, for simplicity we follow the original FKK paper in assuming spin zero projectile, ejectile, and target (Ref. [2] shows how nonzero spins can be included). Also, a variety of numerical MSC calculations have shown that the MSC spectrum is very nearly isotropic for nucleon-induced reactions [6] at the energies we consider here, and therefore we shall present results only for the angle-integrated spectrum. From the above expressions for the fluctuating transition matrix we obtain the cross section for MSC emission as

$$\frac{d\sigma}{dU}=\pi\lambda^2\sum_J(2J+1)\sum_{\mu=0}^{r}\sum_{m=\mu-1}^{\mu+1}\sum_{n=m}^{r}\sum_{\nu=n-1}^{n+1}\sum_{\lambda=\nu}^{r}\sum_{l}\frac{\langle\Gamma_{nJ}^{\uparrow\nu\lambda l}(U)\rangle}{\langle\Gamma_{nJ}\rangle}\left[\prod_{k=m}^{n-1}\frac{\Gamma_{kJ}^{\downarrow}}{\Gamma_{kJ}}\right]\frac{2\pi\Gamma_\mu{}^{(i)}}{D_\mu}, \tag{13}$$

where U is the residual nucleus energy, J is the composite nucleus angular momentum, l is the emitted particle angular momentum, $\langle\Gamma_{nJ}^{\uparrow\nu\lambda l}(U)\rangle$ is the emission width of stage n, and $\langle\Gamma_{nJ}\rangle$ is the total width of stage n. The quantity in the square brackets is the depletion factor, which accounts for flux lost to emission from previous stages, and $2\pi\Gamma_\mu/D_\mu^{(i)}$ is the strength function for entrance into Q space from stage μ.

This equation looks very similar to that of FKK [see, for instance, Eq. (3.41) in Ref. [1]]. But in addition to the sum over preequilibrium stages n, ν already present in the FKK equation, there are summations over (1) μ, the last P stage before Q space is entered; (2) m, the initial Q stage entered; (3) λ, the final P stage from which emission occurs. Physically, initial MSD scatterings in P space are included via the strength function, which is defined for each stage of entrance into Q space (see below). Likewise, subsequent MSD scatterings are included within the definitions of the emission rates, which include the label λ (see below). In the special case of $\mu=0$ and $\lambda=\nu$, Eq. (13) reduces to the original FKK Eq. (3.41) [1], while the other terms in the summations account for linking between MSC and MSD. The above equation is a generalization of the expression given in the appendix of Marcinkowski *et al.*'s paper [8].

As in the original FKK paper, the random phase approximation results in a coherence only between continuum particles with the same direction, resulting in the well-known convolution structure of multistep transitions in the P chain. This enables the strength function for a given stage μ to be expressed as a convolution of one-step MSD probabilities, finally folded into the entrance strength function. Thus, the μth entrance strength function, which describes $P\rightarrow Q$ processes, is given by

$$\frac{2\pi\Gamma_\mu{}^{(i)}}{D_\mu}=\int\frac{d\mathbf{k}_1}{(2\pi)^3}\cdots\frac{d\mathbf{k}_\mu}{(2\pi)^3}\frac{2\pi\Gamma_0{}^{(\mu)}}{D_0}\left[\frac{d^2\omega^{(1)}(\mathbf{k}_\mu\leftarrow\mathbf{k}_{\mu-1})}{dU_\mu d\Omega_\mu}\right]\left[\frac{d^2\omega^{(1)}(\mathbf{k}_{\mu-1}\leftarrow\mathbf{k}_{\mu-2})}{dU_{\mu-1}d\Omega_{\mu-1}}\right]\cdots\left[\frac{d^2\omega^{(1)}(\mathbf{k}_2\leftarrow\mathbf{k}_1)}{dU_2d\Omega_2}\right]\times\left[\frac{d^2\omega^{(1)}(\mathbf{k}_1\leftarrow\mathbf{k}_i)}{dU_1d\Omega_1}\right], \tag{14}$$

where the terms in the square brackets are exactly the same one-step probabilities that are used in the MSD theory. Likewise, we describe transitions in P space that can follow MSC emission as

$$\Gamma_{nJ}^{\uparrow\nu\lambda l}=\int\frac{d\mathbf{k}_\lambda}{(2\pi)^3}\cdots\frac{d\mathbf{k}_\nu}{(2\pi)^3}\left[\frac{d^2\omega^{(1)}(\mathbf{k}_f\leftarrow\mathbf{k}_\lambda)}{dU_f d\Omega_f}\right]\left[\frac{d^2\omega^{(1)}(\mathbf{k}_\lambda\leftarrow\mathbf{k}_{\lambda-1})}{dU_\lambda d\Omega_\lambda}\right]\cdots\left[\frac{d^2\omega^{(1)}(\mathbf{k}_{\nu+2}\leftarrow\mathbf{k}_{\nu+1})}{dU_{\nu+2}d\Omega_{\nu+2}}\right]\left[\frac{d^2\omega^{(1)}(\mathbf{k}_{\nu+1}\leftarrow\mathbf{k}_\nu)}{dU_{\nu+1}d\Omega_{\nu+1}}\right]\Gamma_{nJ}^{\uparrow\nu l}(E_\nu) \tag{15}$$

where $\Gamma_{nJ}^{\uparrow\nu l}(E_\nu)$ is the width for immediate emission. Our numerical calculations of additional rescatterings in P space after emission using Eq. (15) indicate that they are of minor importance. But as we shall show below, $P\rightarrow Q$ transitions [from Eq. (14)] can be very significant. The entrance function $2\pi\Gamma_0/D_0$ in Eq. (14) was calculated microscopically using the approach of Bonetti *et al.* [2], using constant wave functions [1].

We apply our linked MSD-MSC formalism to describe 14 MeV neutron inelastic scattering on niobium, which has become a test case in the literature for theoretical analyses. The calculational approach and input parameters described in Ref. [6] were used in the FKK-GNASH code system [6,13] to obtain the cross sections. Unlike Ref. [6] which estimated the crossover transitions using phase space arguments, we explicitly calculate them with Eqs. (14) and (15). Also, when calculating the multistep processes we use modified DWBA matrix elements, which we denote as "MDW" (sometimes called "non-normal" DWBA in the literature). The MDW matrix elements differ from their corresponding normal DWBA matrix elements by an inverse S-matrix factor. They use the boundary conditions that naturally appear in the complete set of states inserted in the evaluation of the intermediate state optical Green's function, and have been advocated by Kawai and others, and noted recently in Koning and Akkermans' derivation [14].

The residual nucleon-nucleon interaction strength $V_0^{\rm MSD}$ (which affects the magnitude of MSD emission as well as the multistep P-space transitions involved in $P\rightarrow Q$ processes) is treated as a parameter in the theory. We obtained $V_0^{\rm MSD}=36$ MeV by fitting the MSD emission cross section extracted from experimental data [6]. The interaction strength for MSC processes, which enters the overlap integral in the entrance strength function, was obtained from unitarity since the total $P\rightarrow Q$ flux equals the reaction minus the MSD cross section.

In Fig. 2 we show our results for the $P\rightarrow Q$ flux into the compound chain at the various stages m. For comparison we

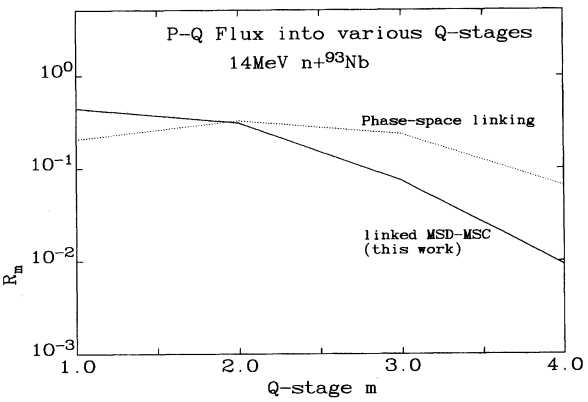

FIG. 2. Fraction of reaction flux entering the Q chain at stage m.

also show the phenomenological phase-space model [6,8] results. R_m denotes the fraction of the reaction cross section that enters the compound chain at stage m. It is evident that $P \rightarrow Q$ transitions beyond the initial $P_0 \rightarrow Q_1$ are significant and absorption into the compound chain is a gradual process. Even though the phase-space estimate does not agree exactly with our theoretical calculations, there is a qualitative agreement insofar as both predict a gradual absorption. Our calculation of the initial $P_0 \rightarrow Q_1$ flux is about twice that predicted by the phase-space model, and in good accord with the results of Sato and Yoshida [11]. Our theory predicts an increasing importance of $P \rightarrow Q$ crossover transitions with increasing incident energy. Indeed, when the incident energy exceeds the sum of the Fermi and binding energies, absorption into the compound chain always take place after a number of P-space transitions.

The angle-integrated emission spectrum from our linked MSD-MSC theory in the 14 MeV ^{93}Nb(n,n') reaction is shown in Fig. 3. The contributions of MSC, MSD, and Hauser-Feshbach processes are indicated. Given that the complete spectrum, and the MSD-MSC linking, is obtained quantum mechanically without any parameter adjustment,

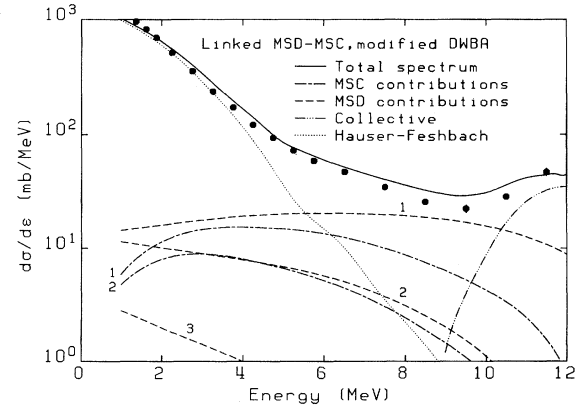

FIG. 3. Linked MSD-MSC theory compared with angle-integrated 14 MeV ^{93}Nb(n,n') data of Pavlik *et al.* [15]. The labels 1,2,3 on the MSD and MSC curves describe contributions from the different preequilibrium stages $P1$,$P2$,$P3$ and $Q1$,$Q2$,$Q3$, respectively.

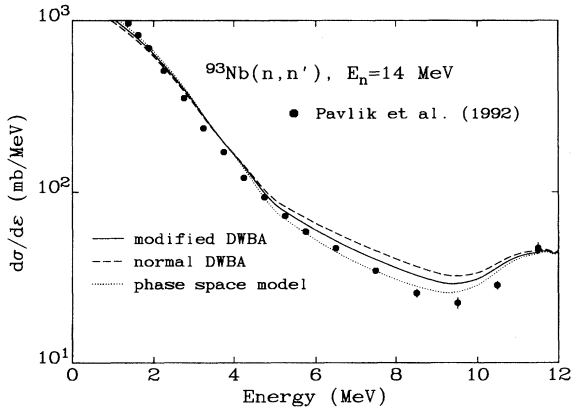

FIG. 4. Linked MSD-MSC theory compared with angle-integrated 14 MeV ^{93}Nb(n,n') data of Pavlik *et al.* [15]. Results obtained with the present theory are shown for both the modified DWBA (MDW) and normal DWBA boundary conditions. Also shown is the result obtained with the phenomenological phase-space model. With increased linking between the P and Q chains, the initial MSC Q stage tends to be bypassed and MSC emission decreases.

the theory describes the measurements rather well. If the theory predicted an even slower absorption into the compound chain the high-energy MSC emission would be further reduced, improving the agreement with data in the 7–10 MeV range. This is because the dominant contribution to MSC comes from the first $2p1h$ stage (Q_1), and bypassing this stage reduces MSC emission. For comparison, we show in Fig. 4 the spectrum when the MSD-MSC linking is achieved using the phenomenological phase-space model [8], with the MDW prescription for MSD emission. This model predicts an even smaller MSC emission (due to the large amount of $P \rightarrow Q$ transitions as shown in Fig. 2) and describes the data well.

For comparison we also performed the linked MSD-MSC theory calculations using the prescription proposed by Feshbach [16] which uses normal DWBA matrix elements in the multistep calculations. But we found that this approach provides a negligibly small amount of $P \rightarrow Q$ transitions (since multistep processes in the P chain are significantly smaller here) and results in a preequilibrium emission spectrum that overpredicts experiment (see Fig. 4). Even though the MDW approach overpredicts the preequilibrium emission spectrum as well, the improvement is readily noticeable. Further details of our experience in using MDW and normal DWBA are given in Ref. [17]. Marcinkowski's article [8] concluded by highlighting one issue—why should the multistep processes involved in $P \rightarrow Q$ transitions be significant if the multistep contributions to MSD emission are very small? Our work addresses this question. We only find significant $P \rightarrow Q$ transitions beyond the initial $P_0 \rightarrow Q_1$ when the multistep MSD contributions are also significant, i.e., when MDW is used.

In summary, we have generalized the FKK theory to include a linking of the P and Q chains which results in three new types of MSC emission. Our work provides a theoretical basis for the presence of processes usually described in the literature by the phase-space model. Without this linking, the

FKK theory overestimates preequilibrium emission. Our theory gives an improved description of measurements, but there is still some excess compared to experimental data. Further improvement may be obtained with more sophisticated calculations.

This work was performed in part under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48, and under Contracts DE-AC02-76ER03069 and DE-FC02-94ER40818.

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