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Preequilibrium spin effects in Feshbach-Kerman-Koonin and exciton models and application to high-spin isomer production

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We describe how the Feshbach-Kerman-Koonin (FKK) theory can be used to obtain residual nucleus spin distributions following preequilibrium decay, by removing the assumption of zero intrinsic spins in multistep direct reactions. By making use of parallels between the exciton model and the FKK multistep direct theory we also obtain a straightforward method for determining spin distributions in the exciton model. We compare these two approaches and apply them to high-spin isomer production cross sections in 14 MeV neutron reactions on hafnium. We obtain reasonable agreement with measurements, though there is evidence that the FKK theory underpredicts high spin transfer reactions. Comparisons with the exciton model suggest that multistep processes in FKK are underestimated, and that an FKK formulation incorporating non-normal DWBA transitions may yield results in closer agreement with the exciton model, and with experiment.

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The quantum mechanical theory of Feshbach, Kerman, and Koonin (FKK) [1] describes inelastic multistep processes in nucleon-induced reactions below about 200 MeV. Its formalism allows a direct calculation of the spin distributions of residual nuclei remaining after preequilibrium emission. The semiclassical exciton model, on the other hand, is usually formulated without the inclusion of spin effects, though there have been a number of works which have addressed such considerations [2, 3]. In this communication we present new techniques for obtaining preequilibrium spin distributions in both the FKK theory and the exciton model, and we compare both models along with their predictions of high-spin isomer production in 14 MeV neutron-induced reactions.

The FKK theory distinguishes multistep compound (MSC) and multistep direct (MSD) preequilibrium reactions, and at incident energies below about 50 MeV both types of reactions contribute. The theory was originally formulated with an assumption of zero intrinsic projectile, ejectile, and target spin (to simplify the angular momentum couplings), though calculations of observables sensitive to spins require a more accurate treatment. The work of Herman *et al.* [4] and Chadwick *et al.* [5] removed this assumption in MSC reactions, which were originally assumed to be dominant at 14 MeV. However, recent analyses indicate that MSD dominates preequilibrium reactions even at energies as low as 14 MeV [6, 7] and thus we show here how nonzero intrinsic spins can be included in MSD calculations.

Following the emergence of quantum mechanical preequilibrium theories there have been a number of works which have sought to elucidate links between such theories and the exciton model [2, 8, 9]. Akkermans and Koning [9] showed that under various assumptions the exciton model can be obtained from the MSD theory. We follow this work by showing how exciton model spin distributions can be obtained by taking advantage of links between the exciton model and FKK MSD theory.

In order to determine the accuracy of these preequilibrium theories, phenomena sensitive to angular momentum effects must be investigated. Our recent work [10] on discrete gamma-ray cross sections in $(n, xn\gamma)$ reactions is one such case where accurate modeling of spin distributions was found to be important. Another phenomenon, which we address in this work, is the production of high-spin isomeric states in neutron reactions. Using both the FKK theory and our exciton model we determine the production of the ^{178m2}Hf(16^+, $t_{1/2}$= 31 years) and the ^{179m2}Hf(12.5^-, $t_{1/2}$=25 days) isomers in 14 MeV neutron reactions on ^{179}Hf. These reactions are of great importance in assessing radioactive waste production in proposed fusion reactors and are currently under investigation by a Coordinated Research Programme of the International Atomic Energy Agency [11].

MSD theory represents an extension of distorted-wave-Born-approximation theory (DWBA) into the continuum, and can be derived from a Lippmann-Schwinger expansion of the transition amplitude [9]. We remove the original FKK spin-zero approximation in MSD by treating the $1p1h$ states excited in the interaction as absorbing the transferred angular momentum, after which their angular momentum couples with the intrinsic "core" spin of the target. This allows us to account for nonzero intrinsic spins while being able to use much of the existing MSD calculational formalism. For projectile and ejectile spins $\mathbf{i}$ and a target spin $\mathbf{I}$, leaving a residual nucleus with spin $\mathbf{J}$ after inelastic scattering with an orbital angular momentum transfer $\mathbf{l}$, we have $\mathbf{J} = \mathbf{I} + \mathbf{i} - \mathbf{i} + \mathbf{l}$ and we write the spin flip as $\mathbf{S_f} = \mathbf{i} - \mathbf{i}$. The 1-step MSD cross section is then given by

$$\frac{d^2\sigma(E,\Omega\leftarrow E_0,\Omega_0)}{d\Omega dE}_{1\text{ step}}=\sum_J\frac{(2J+1)}{(2I+1)(2i+1)}\sum_{S_f=0}^{1}\frac{1}{(2S_f+1)}\times\sum_{S=|I-S_f|}^{I+S_f}\sum_{l=|J-S|}^{J+S}\rho(1p,1h,E_0-E,l)\left\langle\left[\frac{d\sigma(E,\Omega\leftarrow E_0,\Omega_0)}{d\Omega}\right]_l^{\rm DWBA}\right\rangle. \tag{1}$$

In the limit of zero intrinsic spins this expression reduces to the usual FKK 1-step MSD result [6, 12]. Also, in the absence of the averaged DWBA cross sections and the energy-dependent part of the level density, the summation over J yields unity, as in the original FKK case. We have found that using nonzero spins in the MSD calculation can have a large impact on the residual spin distributions (especially if the target spin is large), though the impact on calculated emission spectra is small. The minor influence of spin effects on emission spectra that we find is consistent with similar conclusions by Oblozinsky [2] and by Shi, Gruppelaar, and Akkermans [3] in exciton model studies.

$\rho(1p,1h,E_0-E,l)$ is the density of $1p1h$ states with energy E_0-E and angular momentum l. The density of states for a p-particle, h-hole system can be partitioned into the energy-dependent density multiplied by a spin distribution, $\rho(p,h,E,l)=\omega(p,h,E)\;R_n(l)$. We use the finite-well-depth restricted Williams [13] expression,

$$\omega(p,h,E)=\frac{g^n}{p!h!(n-1)!}\sum_{j=0}^{h}\binom{h}{j}(-1)^j(E-A_{ph}-j\epsilon_F)^{n-1}\times\Theta(E-A_{ph}-j\epsilon_F), \tag{2}$$

where $n=p+h$, and we take the single-particle spacing as $g=A/13$. The Pauli-blocking factor is $A_{ph}=[p^2+h^2+p-3h]/4g$, and ϵ_F is the Fermi energy which we take as 40 MeV. The Θ function is unity if its argument is greater than zero, and zero otherwise. A Gaussian angular momentum distribution is assumed,

$$R_n(l)=\frac{2l+1}{2\sqrt{2\pi}\sigma_n^3}\exp\left[-\frac{(l+1/2)^2}{2\sigma_n^2}\right], \tag{3}$$

with the Gruppelaar-Facchini recommended spin cutoff, $\sigma_n^2=0.24nA^{2/3}$ [14].

$\left\langle\left[\frac{d\sigma(E,\Omega\leftarrow E_0,\Omega_0)}{d\Omega}\right]_l^{\rm DWBA}\right\rangle$ is the average of DWBA cross sections exciting $1p1h$ states of energy E_0-E, consistent with angular momentum and parity conservation. The $1p1h$ states are obtained from a spherical Nilsson model. We calculate the DWBA form factors for the various transitions with DWUCK4 [15] using a Yukawa potential of range 1 fm, and strength V_0. We have used V_0=36 MeV in accordance with systematics developed in our FKK analyses, which, as we shall show in Sec. IV, results in a FKK preequilibrium spectrum close in magnitude to the exciton model, at the higher emission energies. In this calculation, for each 1 MeV energy bin, we average about ten microscopic cross sections for each l transfer, and include nine values of l transfer in Eq. (1) to ensure that all possible $1p1h$ excitation strength is accounted for (and we include microscopic form factors leading to both neutron p-h and proton p-h excitations). When calculating the form factors, unbound-state wave functions were obtained from optical-potential scattering states using the Walter-Guss potential [16], with a Perey-Buck nonlocal range of 0.85 fm, and bound-states from a real Woods-Saxon potential well with radius parameter 1.2 fm and diffuseness 0.6 fm.

Whether MSD multistep cross sections should be obtained from a convolution of normal, or both normal and non-normal, DWBA matrix elements, is still being disputed in the literature [9, 17]. Here we follow Feshbach [17] in using normal DWBA matrix elements, which gives a contribution from the Nth stage,

$$\frac{d^2\sigma^{(N)}(E,\Omega\leftarrow E_0,\Omega_0)}{d\Omega dE}=\frac{m}{4\pi^2\hbar^2}\int d\Omega_{N-1}\int dE_{N-1}E_{N-1}\times\frac{d^2\sigma^{(1)}(E,\Omega\leftarrow E_{N-1},\Omega_{N-1})}{d\Omega dE}\,\frac{d^2\sigma^{(N-1)}(E_{N-1},\Omega_{N-1}\leftarrow E_0,\Omega_0)}{d\Omega_{N-1}dE_{N-1}}, \tag{4}$$

though in Sec. IV we point out some possible problems with this approach.

MSC processes occur when a chain of p-h states is populated in which all the particles are bound. Recent analyses of 14 MeV (n,n') reactions have pointed to the reduced importance of MSC in comparison with MSD, and our calculations for ^{179}Hf(n,xn) confirm this: our angle-integrated MSC spectrum is less than 20% of the MSD spectrum. Since the angular distribution of preequilibrium particles from 14-MeV reactions shows a clear experimental anisotropy, MSD would be expected to be significant. Also, at these energies preequilibrium emission is dominated by 1-step scattering which, from phase space considerations, contains a large MSD component. Full details of the formalism used for our MSC calculations (with nonzero spins) can be found in Refs. [6,18].

A spin-dependent exciton model has been developed by Oblozinsky [2], making use of parallels between the FKK MSC theory and the exciton model. Particle emission rates were derived from detailed balance, and the spin-dependent part of the two-body emission and damping rates were associated with those from the MSC theory. A drawback to this approach is the technically difficult nature of the angular momentum coupling algebra and the time-consuming averaging of all single-particle states which satisfy angular momentum coupling rules. This formalism was recently implemented into the code PEGAS [19], and with this code we investigated the preequilibrium spin distribution and the high-spin isomer production that is predicted. However, as we shall discuss in more detail in a future paper [20], this approach seems to underpredict high-spin populations in (n, n') reactions.

In this work we have sought, instead, to derive exciton model spin distributions by considering links with the FKK MSD theory. This was motivated, by the work of Akkermans and Koning [9], who have discussed how these two models relate to each other, and by recent work that has pointed to the importance of MSD over MSC even at incident energies as low as 14 MeV [6, 7]. Akkermans and Koning showed that exciton and MSD models have in common the use of "leading particle" quantum statistics, the on-shell approximation, and the independent-particle limit. Furthermore, it is possible to see how the cross sections for 1-step and multistep processes in the exciton model can be obtained from the FKK theory. In the case of 1-step emission, if in the FKK theory expression [Eq. (1)] the averaged DWBA matrix element is replaced by an l-independent inverse cross section along with various other phase space factors from applying detailed balance, the exciton model results. Likewise, for multistep cross sections, if one makes this same substitution in Eq. (4), and in addition factorizes the matrix elements into angular- and energy-dependent parts, one again obtains the exciton result. This is because the energy integral in Eq. (4) then reduces to a convolution of $1p1h$ phase spaces, which for N convolutions equals the $NpNh$ phase space [9], which is found in the exciton model.

These considerations suggest that exciton model spin dependence of residual nuclei can be obtained from the FKK MSD results in Eqs. (1) and (4) by (a) replacing the l-dependent DWBA matrix elements by l-independent global energy averaged values (ultimately obtained by detailed balance); (b) assuming an energy-angle factorization of the DWBA matrix elements; and (c) realizing that the resulting convolution of $1p1h$ densities yield $NpNh$ densities. This leads to a very simple conclusion: the exciton model spin distribution of residual nuclei from a preequilibrium stage N, $P_N(J)$, can be estimated as

$$P_N(J) = \frac{(2J+1)}{(2I+1)(2i+1)} \times \sum_{S_f=0}^{1} \frac{1}{(2S_f+1)} \sum_{S=|I-S_f|}^{I+S_f} \sum_{l=|J-S|}^{J+S} R_n(l), \qquad (5)$$

where $n = p + h = 2N$ and the notation follows that of Eq. (1), and $\sum_J P_N(J)=1$. If the FKK assumption of zero spins is made, this reduces to $P_N(J) = (2J+1)R_n(J)$. But using exact spins, and in particular coupling in the target spin, results in a spin distribution boosted to higher spins than obtained with the zero-spin approximation.

Our calculations use the exciton model of Kalbach [21] combined with Eq. (5) to obtain the spin distributions of residuals following preequilibrium decay. We used default parameters: namely, the damping matrix element was taken as 150 MeV^3 and the single-particle level densities as $A/13$ MeV^{-1}.

In order to compare and test these two models we use them, along with compound nucleus and direct reaction theories, to calculate neutron-induced reactions on ^{179}Hf leading to isomeric states. The two different preequilibrium models (FKK and exciton) are incorporated into the FKK-GNASH [6] and GNASH [21] codes, respectively.

Compound nucleus decay occurs in cases where the chain of particle-hole states reaches equilibrium without undergoing preequilibrium emission. It also accounts for the decay of residual nuclei left in excited states after preequilibrium (or equilibrium) emission. We use the Hauser-Feshbach theory to describe compound nucleus decay, which conserves angular momentum and parity in the reaction. Our calculations follow closely those of our earlier work on hafnium [22]. In brief, the Gilbert-Cameron [23] level density model with pairing energies from the Cook systematics [24] was used to describe the continuum states, and matched on to observed low-lying discrete levels. Rotational bands of experimentally undetected states were built upon the 16^+, 14^- levels in ^{178}Hf and the 12.5^- level in ^{179}Hf, and embedded within the continuum states. Gamma-ray transmission coefficients were calculated with the generalized Lorentzian model of Kopecky and Uhl [25]. The coupled-channel optical potential developed and checked against elastic and total scattering cross sections in Ref. [22] was used.

In Fig. 1 we show the neutron emission spectrum for ^{179}Hf(n, xn) calculated with both the FKK and the exciton models. The two models have similar preequilibrium spectras at higher emission energies, but the FKK spectra is significantly smaller at low emission energies. As we discuss below, this is because the multistep contributions in the FKK theory are smaller than those in the exciton model. When we compare the spin distributions of residual nuclei after preequilibrium emission (Fig. 2), the exciton model distribution is seen to extend to higher values than the FKK distribution. As discussed earlier, the exciton model residual nucleus spin distribution was obtained solely from phase space. Our FKK distribution is the sum of the separate MSC and MSD distributions. The spin distribution from the MSD theory rests upon both the strength of microscopic DWBA transition exciting p-h states for various spin transfers and the p-h phase space [see Eq. (1)]. We found that the MSC spin distribution was rather similar in shape to that of our

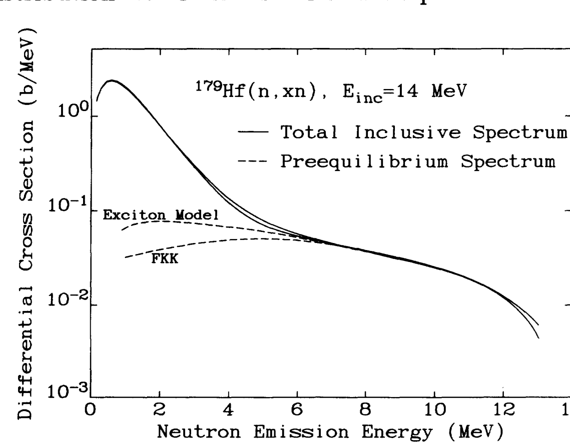

FIG. 1. Comparison of total and preequilibrium neutron emission spectra in $n+^{179}$Hf using FKK and exciton preequilibrium models.

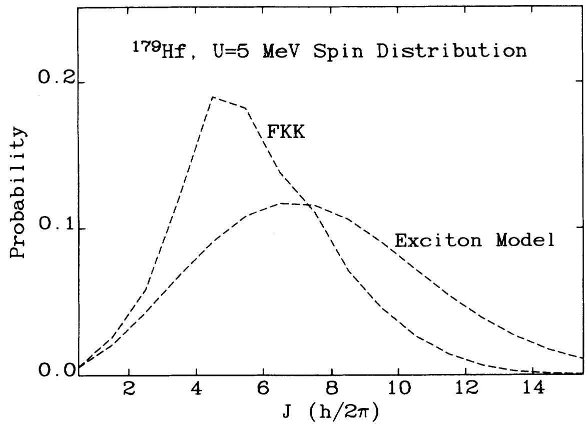

FIG. 2. Comparison of residual nucleus spin distribution at an excitation energy of 5 MeV in ^{179}Hf using FKK and exciton preequilibrium models.

exciton model, though the overall small contribution of MSC compared to MSD resulted in the FKK distribution being dominated by MSD.

In Table I we compare FKK and exciton model calculations with experimental data [27, 28]. The different spin distributions obtained using FKK and exciton models leads to significantly different isomer cross sections. The theoretical calculation of high-spin isomer cross sections is notoriously difficult [22, 26], and uncertainties in the optical model and in the nuclear structure result in theoretical uncertainties of about a factor of 2 to 3 [22]. Given these uncertainties, the calculations (using both FKK theory and the exciton model) are in reasonable agreement with the measurements, though the FKK values, particularly for the (n,n') reaction, are somewhat low. However, the experimental value for the (n,n') reaction was obtained in conjunction with a theoretical calculation, and the reported experimental uncertainty is probably underestimated [28]. Our new calculations using the exciton model agree better with measurements than those we presented in our earlier work [22], which assumed the same spin distribution after preequilibrium and equilibrium decay.

By considering the microscopic DWBA cross sections in the FKK calculation we can determine why the spin distribution after FKK preequilibrium emission is small at high spins. For the case of a residual energy of 5 MeV, as shown in Fig. 2, we find particularly strong DWBA cross sections for l transfers of 1 and 3. In the case of l-transfer=1, this is due to particularly strong transitions exciting the neutron p-h state $2d3/2-2f5/2$ and the proton p-h state $2p1/2-2d3/2$. These strong low l-transfer transitions, when coupled in with the ground-state spin of 4.5, yield residual nucleus spin distributions which are large near 4.5, and smaller for high spins, as seen in Fig. 2.

Our approach to determining the averaged MSD cross section for a given l-transfer follows that of other works, and is as follows: One averages a sample of basic DWBA cross sections and multiplies the average by a spin-dependent level density. A more accurate averaging procedure would be to omit the usual level density term and instead determine all DWBA transitions, multiplying by the number of possible states for each transition, obtained from a deformed Nilsson scheme. Such an improved averaging procedure, while computationally more involved and computer-intensive, may enhance the contributions from high-spin transfer processes. Another possibility for enhancing high-spin transitions in the FKK theory is that multistep MSD cross sections should, perhaps, be determined with a convolution of both normal and non-normal DWBA matrix elements [1, 9], instead of using Eq. (4). This would result in a larger contribution from multistep processes, populating higher spins, and would partly remove the discrepancy. In the present calculations at a 5 MeV residual nucleus energy the FKK 2-step contribution is 3% of the 1-step, compared to 17% found in the exciton model. Our preliminary calculations [29] indicate that an FKK calculation which uses both non-normal and normal DWBA matrix elements yields multistep contributions close to those found in the exciton model, since multistep contributions are enhanced when the non-normal boundary conditions are used. While this enhancement seems to improve the comparisons with data in 14 MeV reactions, the influence on reactions at higher energies still needs to be checked. Our present investigation does suggest that the non-normal theory works well at 14 MeV, but many additional computational checks need to be performed before the non-normal theory can be recommended with confidence.

To summarize, we have presented a MSD formalism which accounts for nonzero spins, and have developed a new and easily applicable method for including spin effects in the exciton model. With these two models we obtain high-spin isomer production cross sections in reasonable agreement with measurements, though there is evidence that the FKK theory underpredicts high spin transfer reactions. Comparisons with the exciton model suggest that multistep processes in MSD are underestimated, and that an FKK formulation including non-normal DWBA transitions may yield results in closer agreement with the exciton model, and with experiment. We are currently investigating modifications to the FKK statistical averaging procedure, and use of a non-normal DWBA formulation, and shall report [20] on their im-

TABLE I. Theoretical 14 MeV neutron-induced cross sections for the production of isomeric states in hafnium compared with experimental data.

Reaction	FKK Preeq. (FKK-GNASH code)	Exciton Preeq. (GNASH code)	Experiment
^{179}Hf$(n,2n)^{178m2}$Hf(16^+)	2.33 mb	10.82 mb	6.29 ± 0.35 mb [27]
^{179}Hf$(n,n')^{179m2}$Hf(12.5^-)	2.93 mb	15.23 mb	12.8 ± 1.5 mb [28]

pact on a range of nuclear reactions sensitive to angular momentum effects.

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