

GEMINI: A Code to Simulate the Decay of a Compound Nucleus by a Series of Binary Decays

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Abstract

The details of the statistical-model code GEMINI are discussed. It is shown that GEMINI does a reasonable job at reproducing experimental charge distributions for light compound nuclei. However for heavier systems, it overpredicts the width of the fission mass distribution. A new code GEMINI++ has been written to address this problem.

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INTRODUCTION

The statistical-model code GEMINI was written in 1986 to address complex-fragment emission in fusion reactions. It differed from most other statistical-models codes at the time in that it allowed not just light-particle evaporation and symmetric fission, but all possible binary-decay modes. Soon after the discovery of fission, Bohr and Wheeler borrowed the one-dimensional transition-state formalism from the study of chemical reaction rates and applied it to symmetry fission [1]. Moretto [2] generalized this formalism by adding an extra dimension associated with mass-asymmetry thus allowing it to treat binary decays of intermediate mass asymmetry. This formalism, in conjugation with barriers calculated for asymmetric fission by Arnie Sierk [3], was incorporated into GEMINI. With these ingredients, GEMINI produced rather good agreement with complex-fragment or asymmetric fission data obtained with light compound nuclei [4-6].

GEMINI is a Monte Carlo code which follows the decay of a compound nucleus by a series of sequential binary decays until such decays are impossible due to energy conservation or improbable due gamma-ray competition. For the latter, only the statistical emission of $E1$ and $E2$ gamma rays is considered, but these are only important at the lowest thermal energies when the particle decay width approaches zero.

As GEMINI was written to confront data from heavy-ion induced fusion reactions, the effects of large angular momenta were explicitly treated. For this reason the dichotomy between light-particle evaporation and other binary decays was still maintained. The best way of treating light-particle evaporation at high angular momentum is via the Hauser-Feshbach formalism [7]. Thus GEMINI differs from most other statistical-model codes used for modeling spallation reactions in that it uses this formalism rather than the Weisskopf-Ewing result [8]. The cost of this better treatment of angular momentum is increased CPU time. The usefulness of this aspect of GEMINI in modeling spallation reactions therefore depends on the degree to which residues with high spin are produced in the initial stages of the reaction. Angular momentum effects include anisotropic angular distributions, although these distributions still process a symmetry about $\theta_{cm}=90^\circ$. To model these correctly, the input to GEMINI must also include the orientation of the spin axis of the excited residue.

For heavy systems, GEMINI simulations generally overpredict the width of the fission mass and charge distributions. Although this may be a failure of the asymmetric fission barriers used in the calculations, it probably signifies a failure of the underlying model. The Moretto formalism predicts the mass-asymmetry distributions along the ridge of conditional saddle points. However, the final mass of the fission fragments is not frozen until the scission point is reached. For light nuclei, the saddle and scission points are almost degenerate so substantial modification during the saddle-to-scission motion is expected to be small. On the other hand for heavy systems, the saddle and scission configurations are quite different. Specifically for very heavy systems, the saddle point can no longer be approximately by two nascent fragments connect by a neck. The neck disappears and the saddle point is a deformed mononucleus and thus one cannot even define an asymmetry degree of freedom. In such cases, the mass asymmetry develops during the descent from saddle to scission. Therefore, the failure of GEMINI for these heavier systems was not unexpected.

Due to these deficiencies of the original code for heavy nuclei, a new code GEMINI++ has been written to address these problems. The new code also signals a change in language. The original version was written in Fortran77 and subsequently changed to Fortran90. The new version, GEMINI++, is written in the C++ language. In addition, a change of philosophy was made. The original GEMINI was written with lots of options to explore changes in the decay characteristics induced by the inclusion of different physics. No effort was made to systematize parameters to obtain a good overall agreement with data from a large range of compound-nucleus masses. In GEMINI++, extensive comparisons with heavy-ion induced fusion data have been used to optimize the default parameters of the model. Such data are useful for constraining statistical-model codes, as unlike spallation, the excitation energy and spin distributions of the compound nuclei can be well defined.

However, this optimization is only for the regions of spin and excitation energies populated by heavy-ion fusion reaction which may not coincide with those produced in spallation.

The details of the various aspects of the two codes are given in the following sections.

LIGHT-PARTICLE EVAPORATION

In the Hauser-Feshbach formalism [7], the partial decay width of a compound nucleus of excitation energy E^* and spin S_{CN} for the evaporation of particle i is

$$\Gamma_i^{HF} = \frac{1}{2\pi\rho(E^*, S_{CN})} \int d\varepsilon \sum_{S_d=0}^{\infty} \sum_{J=|S_{CN}-S_d|}^{S_{CN}+S_d} \sum_{\ell=|J-S_d|}^{J+S_d} T_\ell(\varepsilon) \rho(E^* - B_i - \varepsilon, S_d) \quad (1)$$

where S_d is the spin of the daughter nucleus, S_i , J , and ℓ , are the spin, total and orbital angular momenta of the evaporated particle, ε and B_i are its kinetic and separation energies, T_ℓ is its transmission coefficient or barrier penetration factor, and ρ and ρ_{CN} are the level densities of the daughter and the compound nucleus, respectively. The summations include all angular momentum couplings between the initial and final states which are computationally expensive. Evaporation channels include n , p , d , t , ^3He , α , ^6He , and ^6Li fragments. For the heavier fragments, we include in addition all their excited states with excitation energy less than 5 MeV.

Separation energies B_i , nuclear masses, shell ΔW and pairing ΔP corrections are obtained from the tabulations of Möller *et al.* [9]. Where available the experiment masses are used, otherwise the Finite-Range Droplet model values with shell and pairing corrections are taken.

Transmission coefficients have traditionally been obtained from the inverse reaction using the optical-model parameters obtained from global optical-model fits to elastic scattering data. Alexander *et al.* [10] have pointed out that such transmission coefficients contain the effects of transparency in the inverse reaction which is not appropriate in evaporation. We have therefore kept the real optical-model potentials, but to ensure full absorption, used the incoming-wave boundary-condition model (IWBC) [11] to calculate T_ℓ . Global optical-model potentials were obtained from Refs. [12-18].

The transmission coefficients define the shape of the low-energy or “sub-barrier” region of the evaporation spectra. For α and heavier particles, these IWBC transmission coefficients systematically underpredict the yield of low-energy particles [19-26]. While adjusting the optical-model parameters to reduce the Coulomb barrier can reproduce some of the α -particle data, Li and Be spectra clearly show the need to a distribution of Coulomb barriers [27]. The origin of this distribution may have contributions from compound-nucleus thermal shape fluctuations [28,29] and/or fluctuations in the diffuseness of the nuclear surface. If the fluctuations are thermally induced, then we expect their variance to be proportional to temperature. In GEMINI++, a simplistic scheme was implemented to incorporate the effects of barrier distributions. The transmission coefficients were calculated as

$$T_\ell(\varepsilon) = \frac{T_\ell^{R_0-\Delta r}(\varepsilon) + T_\ell^{R_0}(\varepsilon) + T_\ell^{R_0+\Delta r}(\varepsilon)}{3} \quad (2)$$

which is the average of three IWBC transmission coefficients calculated with three different radii for the nuclear potential. The radii R_0 is the value from the global optical-model fits and $\Delta r = w\sqrt{T}$, consistent with thermal fluctuations. The value of the parameter $w=0.9$ fm was obtained from fits to experiment data.

Nuclear level densities were taken as a Fermi-gas form, i.e.

$$\rho(E^*, J) \propto (2J+1) \exp[2\sqrt{a(U, J)U}] \quad (3)$$

where a is the level-density parameter and the thermal excitation energy $U = E^* - E_{rot}(J) + \delta P$ is back shifted by the pairing correction δP and the rotational energy of the ground-state configuration $E_{rot}(J)$. The latter is taken from the Finite-Range model of Sierk [30].

Following Ignatyuk *et al.* [31,32], the fade out of shell effects is included in the level-density parameter as

$$a(U) = \tilde{a}(U) \left[1 + h(U) \frac{\delta W}{U} \right] \quad (4)$$

where the function specifying the rate of fade out is

$$h(U) = 1 - \exp(-\eta_1 U). \quad (5)$$

The fadeout parameter was set to $1/\eta_1 = 18.5$ MeV [31-32].

From neutron resonance counting, one finds that at low excitation energies $\tilde{a} \cong A/7.3$ MeV [31]. At higher excitation energies probed by fusion reactions, smaller values are needed to reproduce the kinetic-energy spectra of evaporated particles. Thus \tilde{a} must be dependent on the excitation energy. A number of studies [25,26,33] have assumed the form

$$\tilde{a}(U) = \frac{A}{k + \kappa \frac{U}{A}} \quad (6)$$

where k and κ can be obtained from fits to data and the κ term can be thought of as a first order correction to a constant value of k . For Yb compound nuclei where evaporated n , p , and α spectra were fit, values of $k=7$ MeV and $\kappa=1.3$ MeV were obtained [33]. For heavier systems, where only p , and α spectra were available, not unique values of k and κ were obtained from fits, but if $k \approx 8$ MeV is assumed, then κ values of 3 MeV for ^{193}Tl [26], 2-3 MeV for ^{200}Pb [25], 4.3 MeV for ^{213}Fr [26], and 8.5 MeV for ^{224}Th [26] compound nuclei were deduced. In addition for ^{106}Cd compound nuclei, evaporation spectra were well reproduced up to high excitation energies with a constant $\tilde{a} = A/7.5$ MeV, i.e. $\kappa=0$. These results suggest that κ increases rapidly with A . To systematize this effect in GEMINI++, these data and other evaporation spectra were fit with a slightly different form which was felt to have a better asymptotic behavior,

$$\tilde{a}(U) = \frac{A}{k_\infty - (k_\infty - k_0) \exp\left(-\frac{\kappa}{k_\infty - k_0} \frac{U}{A}\right)}. \quad (7)$$

At $U=0$, $\tilde{a} = A/k_0$ where $k_0=7.3$ MeV from neutron resonance counting. For low values of U/A , this form reduces to the previously form of Eq. 6. The evolution of the level-density parameter with excitation energy is thought to be associated with the washing out of long-range correlations associated with coupling between nucleon degrees of freedom and surface vibrations. In the ground state, these long-range correlations cause the single-particle level density $g(\varepsilon)$ to be enhanced near the Fermi energy ε_F [34]. Now as $\tilde{a} \propto g(\varepsilon_F)$, so the washing out of these correlations reduces its value. The level-density parameter should therefore approach the value with no correlations which was taken as $\tilde{a} = A/k_\infty$ ($k_\infty=12$ MeV). Experimental evaporation data can be reproduced with $\kappa = 0.00493 \exp(0.0332A)$.

This strong mass dependent has significant consequences for fission of the heavier systems (see later).

The angular distributions of the evaporated fragments can be determined from the ℓ and m quantum numbers of the evaporated particles. One must provide the initial spin projection of the compound nucleus and then use Clebsch-Gordan coefficients and the predicted values of J , ℓ , and S_d to determine the m distributions of the emitted fragment. Although such an approach is implemented in GEMINI for evaporation only, we lack a quantum-mechanical model to follow the m -state distributions through fission. A more general procedure is to use a quasi-classical approach which is also implemented in GEMINI and is the only option is GEMINI++. From the values of J , ℓ , and S_d predicted by the Hauser-Feshbach formalism and the initial spin alignment of the parent nucleus, a

classical vector associated with ℓ is determined. The angular distribution of the evaporated particle about this vector is then chosen from the distribution $\frac{dN}{d\Omega} = |P_\ell^\ell(\cos\theta)|^2$.

FISSION AND COMPLEX FRAGMENT DECAY

The Bohr-Wheeler transition-state decay width for symmetric fission [2] is

$$\Gamma_{BW} = \frac{1}{2\pi\rho_{CN}(E^*, S_{CN})} \int d\varepsilon \rho_{sad} [E^* - B_f(S_{CN}) - \varepsilon] \quad (8)$$

where ρ_{sad} is the level-density at the saddle-point, $B_f(S_{CN})$ is the spin-dependent saddle-point energy (fission barrier + ground-state rotational energy) and ε is the kinetic energy in the fission degree of freedom. The 2-dimension extension of this by Moretto is

$$\Gamma(y)dy = \frac{1}{2\pi\rho_{CN}(E^*, S_{CN})} \iint \frac{dy dp_y}{h} d\varepsilon \rho_{sad} \left[E^* - B(y, S_{CN}) - \frac{p_y^2}{2m_y} \varepsilon \right] \quad (9)$$

where y is the mass asymmetry, p_y is its conjugate momentum, m_y is the inertia associated with motion in the y coordinate, and $B(y, S_{CN})$ are the energies of the condition saddle-points. The barriers are conditional in the sense they represent a saddle-point configuration when the specified mass-asymmetry is imposed. In the potential-energy surface, these conditional saddle points represent a ridge which must be crossed in order to arrive at the scission configuration.

Simplification to this formula can be made from the expansion

$$\rho(E^* - x) \cong \rho(E^*) \exp\left(-\frac{x}{T}\right) \quad (10)$$

where the nuclear temperature is determined as

$$\frac{1}{T} = \frac{d \ln \rho(E^*)}{dE^*}. \quad (11)$$

With this expansion, the above equation can be reduced to

$$\Gamma(y)dy = \frac{1}{2\pi\rho_{CN}(E^*, S_{CN})} \frac{\sqrt{2\pi T m_y}}{h} \int d\varepsilon \rho_{sad} [E^* - B(y, S_{CN}) - \varepsilon] \quad (12)$$

With this formalism, in addition to the conditional barriers, one also requires knowledge of the inertia m_y . Later Moretto suggest a new formalism [35]

$$\Gamma_Z = \frac{1}{2\pi\rho_{CN}(E^*, S_{CN})} \int d\varepsilon \rho_{sad} [E^* - B_Z(S_{CN}) - \varepsilon] \quad (13)$$

where here Z is the proton number of one of the nascent fragments. Basically the term $\frac{\sqrt{2\pi T m_y}}{h}$ has been eliminated and the problem has been discretized. In GEMINI this was further extended by allowing for distinct mass and charge splits:

$$\Gamma_{Z,A} = \frac{1}{2\pi\rho_{CN}(E^*, S_{CN})} \int d\varepsilon \rho_{sad} [E^* - B_{Z,A}(S_{CN}) - \varepsilon] \quad (14)$$

The conditional barriers now have both the mass and charge asymmetries imposed and are estimated as

$$B_{Z,A}(S_{CN}) = B_A^{Sierk}(S_{CN}) + \Delta M + \Delta E_{Coul} - \delta W - \delta P \quad (15)$$

where δW and δP are the ground-state shell and pairing corrections to the liquid drop barrier. Shell and pairing effects at the conditional saddle points are assumed to be small. The quantity B_A^{Sierk} is the interpolated Sierk barrier for the specified mass asymmetry. In the Sierk's Finite-Range calculations,

the two nascent fragments have the same Z/A ratio. The correction ΔM now accounts for the different Z/A values of the two fragments, i.e.

$$\Delta M = M(Z, A) + M(Z_{CN} - Z, A_{CN} - A) - M\left(Z_{CN} \frac{A}{A_{CN}}, A\right) - M\left(Z_{CN} \frac{A_{CN} - A}{A_{CN}}, A_{CN} - A\right) \quad (16)$$

where $M(Z, A)$ is the spherical Finite-Range Model mass. In addition there is Coulomb correction

$$\Delta E_{Coul} = E_{Coul}(Z, A, Z_{CN} - Z, A_{CN} - A) - E_{Coul}\left(Z_{CN} \frac{A}{A_{CN}}, A, Z_{CN} \frac{A_{CN} - A}{A_{CN}}, A_{CN} - A\right) \quad (17)$$

where $E_{Coul}(Z_1, A_1, Z_2, A_2)$ is the Coulomb energy between two fragments (Z_1, A_1) and (Z_2, A_2) estimated as two spheres separated by 2 fm with a radius parameter of 1.225 fm.

The total width requires summations over both the Z and A values of the lightest fragment.

This formalism was implemented with spin-dependent conditional barriers $B_A^{Sierk}(S_{CN})$ interpolated from the Sierk's full finite-range model calculations for ^{110}In [3], ^{149}Tb [36], and ^{194}Hg and, for lighter systems, from Sierk's finite-range calculations using a more simplistic two-spheroid shape parameterization. In the latter case, all barriers were scaled such that the symmetric barrier was consistent with the full finite-range model value. For systems which are more fissile than ^{194}Hg , the ^{194}Hg barriers are used.

This scheme works well for light systems which have a minimum in the mass distribution of the decay products for symmetric division. In these cases the saddle and scission point are almost degenerate. For heavier compound nuclei, saddle and scission points are also still expected to be approximately degenerate for asymmetric divisions [37]. Therefore in GEMINI++, for both light systems and for asymmetric divisions of heavy systems, the Moretto formalism is kept. All binary divisions are included which have asymmetries greater than the value at which the conditional barrier is a minimum, which is spin dependent.

For the more symmetric divisions in heavy nuclei, the Bohr-Wheeler formalism is used to predict the total symmetric fission yield in GEMINI++. The fission barrier is taken from Sierk's Finite-Range Model value after correcting for the ground-state shell and pairing correction, i.e.,

$$B_f(S) = B_f^{Sierk}(S) - \delta W - \delta P. \quad (18)$$

With the parameterized excitation-energy dependent level-density parameters, we find excellent agreement with experiment fission cross sections if the Bohr-Wheeler width is scaled by the factor 2.4 and the ratio of level-density parameters a_f/a_n for the saddle and ground state configuration is taken as unity. One can also obtain similar agreement if the Sierk fission barriers are reduced or if a_f/a_n is increased. The level-density formalism used in GEMINI++, predicts large enhancements in the residue cross section produced in very heavy nuclei where fission is the dominant decay mode. With a constant level-density parameter, residue cross sections are expected to be small in such nuclei. With the excitation-energy dependent level-density parameters, fission is still dominant, but the residue cross sections, though still small, are greatly enhanced. Such enhancements are observed experimentally and were previously explained by dissipation and fission delays. The present analysis suggests a much smaller role for the dependence of the fission probability on these dissipative effects and thus they are not included in the default mode of GEMINI++.

However, friction is not forgotten. Once the saddle-point is crossed, the system losses excitation energy due to light-particle evaporation during the slow saddle-to-scission motion. To estimate the magnitude of this effect, the time required for this motion was assumed to be $t = \eta (B_{sad} - B_{sciss})$ where B_{sad} and B_{sciss} are the symmetric saddle and scission point energies and η is the friction. The scission-point energy is determined as $B_{sciss} = Ek^{tot} - Q_f$ where Ek^{tot} is the total kinetic energy released in fission from Ref. [38] and Q_f is fission Q value. In the descent from saddle to scission, excitation energy is being increased due to dissipation and at the same being lost due to evaporation. Significant CPU time would be required to fully model this process, so instead a simple formalism was adopted. As the total number of neutrons emitted is largely determined from the statistical lifetime of the last emitted

particle, we only consider evaporation from the scission-point configuration. The total change in potential between saddle and scission $B_{sad}-B_{sciss}$ is assumed to be dissipated into excitation energy at the scission point. As B_{sciss} is spin independent, the Weisskopf-Ewing formalism is used for evaporation at this stage to calculate the decay widths, i.e.,

$$\Gamma_i^{WE} = \frac{(2S_i + 1)}{2\pi\rho_{sciss}^0(E^*)} \int \frac{2\mu\epsilon\sigma_{inv}(\epsilon)}{\pi\hbar^2} \rho_{sciss}(E^* - \epsilon) d\epsilon \quad (19)$$

where μ is the reduced mass, σ_{inv} is the inverse cross section, and

$$\frac{2\mu\epsilon\sigma_{inv}(\epsilon)}{\pi\hbar^2} = \sum_{\ell=0}^{\infty} (2\ell + 1) T_{\ell}(\epsilon). \quad (20)$$

The transmission coefficients of Eq. 2 are used, although, in principle, as we are now dealing with evaporation from a deformed system, the Coulomb barriers for charged-particle emissions should be lowered. However as charge-particle multiplicities are expected to be small, this is not a large problem. The quantities ρ_{sciss}^0 and ρ_{sciss} are the spin-independent level densities of the parent and daughter;

$$\rho_{sciss}(E^*) \propto \exp[2\sqrt{a(E^* - B_{sciss})}] \quad (21)$$

where a level-density parameter of $a = A/8$ MeV was assumed. From fitting systematics of prefission neutrons multiplicities [39] one obtained $\eta=2$ zs/MeV.

Finally, the systematics of fission mass distributions compiled by Rusanov *et al.* [38] are used to choose the mass division from the final scission temperature. Once a binary division has been selected, it is important to find the emission angle and the spins of the fragments. These are selected from the statistical treatment of angular-momentum bearing normal modes such as bending, wriggling, tilting and twisting developed by Moretto [40] and subsequently extended to asymmetric mass division by Schmitt and Pacheco [41]. Thermal fluctuations are considered in the subdivision of the total thermal excitation energy U_{tot} between the two fragments, i.e., the probability is

$$P(U_1) \propto \exp(2\sqrt{a_1 U_1}) \exp[2\sqrt{a_2 (U_{tot} - U_1)}] \quad (22)$$

where U_1 is the thermal excitation energy of one fragments and a_1 and a_2 are the level-density parameters of each fragment.

GAMMA-RAY EMISSION

At very low excitation energies, the partial decay widths for particle and gamma decay can be comparable and thus it is important to include gamma-ray emission to correctly model the termination of particle decay. However for this purpose only the $E1$ and $E2$ gamma rays need be considered. From Blatt and Weisskopf [42], the decay width for multipolarity ℓ is

$$\Gamma_{\gamma}^{\ell} = F_{\ell} \frac{18(\ell + 1)}{\ell(\ell + 3)^2 [(2\ell + 1)!]^2} \frac{e^2}{\hbar c} \left(\frac{R}{\hbar c} \right)^{2\ell} \frac{1}{D_0} \sum_{s_d = |S_{CN} - \ell|}^{S_{CN} + \ell} \int \epsilon^{2\ell + 1} \frac{\rho(E^* - \epsilon, S_d)}{\rho(E^*, S_{CN})} d\epsilon \quad (23)$$

where ϵ is the gamma-ray energy, $R = 1.2A^{1/3}$ fm, D_0 is 1 MeV, and F_{ℓ} accounts for deviations from the Weisskopf estimates. Values of $F_1=0.025$ and $F_2=9.0$ were taken from Ref. [43].

CONCLUSION

The statistical-model code GEMINI follows the decay of a compound nucleus by a series of binary divisions. The partial decay widths are taken from the Hauser-Feshbach formalism for light-particle evaporation and from Moretto's generalized transition-state formalism for more symmetry divisions. This prescription provides an adequate description of the decay process for light compound nuclei. For heavier systems, the predicted mass distributions are too wide. A new code GEMINI++, was written to overcome this problem. For heavy systems, the Bohr-Wheeler formalism is now used for symmetric fission and the width of the mass distributions of the fission fragments is interpolated from systematics.

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