Configuration mixing in pre-equilibrium reactions

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We present a unified semiclassical model of nucleon-induced pre-equilibrium reactions that permits the simulation of varying degrees of internal configuration mixing. We use it to compare the case of no configuration mixing with that of complete mixing. We also compare the two with an intermediate case that we call the natural model. The no-mixing and natural models yield very similar results, which are quite different from the complete-mixing ones. To reproduce standard exciton model spectra, the model simulations require complete mixing and an intraclass transition rate that is a thousand times larger than the natural one.

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I. INTRODUCTION

Pre-equilibrium emission plays an ever more important role in nucleon-induced reactions as the incident energy increases above about 10 MeV. Models that describe such reactions were developed long ago. The first of these was the intranuclear cascade model, which follows sequences of two-body collisions through the spatial volume of the nucleus [1-3]. Elaborations on this model continue to be widely used for the description of high-energy reactions [4-6]. A different approach was introduced by Griffin, who described a pre-equilibrium reaction in terms of a sequence of collisions that populate increasingly complex configurations of single-particle excitations, thus transferring the cascade from geometrical space to energy space [7]. The two best-known semiclassical pre-equilibrium models, the hybrid [8-10] and exciton models [11–15], are based on such an approach. An appealing feature of these models is that they assume the population of all possible configurations of a given class to be equally likely, so that particle emission can be estimated simply on a statistical basis. Although more sophisticated quantum mechanical models have been developed over the years [16–23], many calculations for technological applications still rely on these older, but very successful, semiclassical models [24-26].

The differences between the hybrid and exciton models were a point of contention for many years. Bisplinghoff [27] argued that the fundamental differences between the two are their assumptions concerning the degree of mixing among configurations with the same number of particles and holes. While the hybrid model assumes that no configuration mixing occurs at all, the exciton model assumes the mixing to be such that the configurations in each class are equally populated at each stage of the collison. Bisplinghoff went on to show that the exciton (quasiparticle) state densities used in the two models are quite different from the distributions expected from scattering to still more complicated exciton configurations, except in the cases of the very simplest densities. His analysis thus fell hardest on the hybrid model, since its use of these exciton densities is difficult to reconcile with the assumption of no configuration mixing. The exciton model, by assuming the equal occupation of all configurations in a class, has reason to use them, although the question

of how such equal occupations might be attained was left unanswered.

A decade later, Blann proposed an alternative to the hybrid model, called the hybrid Monte Carlo simulation (HMS) model [28,29], which uses only those lowest-order exciton densities that are consistent with the kinematics of nucleonnucleon scattering in a nucleus [10]. The HMS model, like the hybrid model, contains no configuration mixing but is now conceptually consistent with that hypothesis. As stated in its name, the HMS model uses a Monte Carlo simulation method to obtain results. This puts it at a disadvantage in computational terms when compared with the hybrid and exciton models, in which the use of exciton state densities permits simple, rapid calculations. However, contrary to the hybrid model, the HMS presents a conceptually consistent alternative to the exciton model, but with the same hypothesis of no configuration mixing used in the original hybrid model.

In the following, we extend a framework very similar to that of the HMS model to one that can simulate the exciton model as well. Our aim is to compare the hypotheses of the two models within this unified basis. We do not compare calculations to experimental data because the capacity of the two to fit the data, after model parameters have been fine tuned, is well known. Rather, we compare them with each other for the same parameter values and analyze their internal conceptual consistency.

Since our objective is not the description of experimental data, we develop the unified model in its simplest form. We do not distinguish between neutron and protons, nor do we consider any of the other refinements and extensions of the hybrid, HMS, and exciton models, such as the calculation of angular distributions [29–31] or the inclusion of the effects of the nuclear surface [9], of angular momentum conservation [32], or of cluster emission [33–40], among others.

In Sec. II, we discuss the general hypotheses on which the HMS and exciton models are based, as well as the hypotheses particular to each of the two. We describe the unified model in Sec. III. There, we also define a "natural" model as a special case and show that the fundamental hypotheses of the HMS and exciton models are obtained in limiting cases of the model. In Sec. IV, we present numerical results for the emission

spectra and multiplicity distributions of the different models. We conclude in Sec. V.

II. THE HMS AND EXCITON MODELS

Semiclassical pre-equilibrium models are usually formulated on the basis of a set of independent single-particle states of the composite nucleon-nucleus system. In the ground state of the system, all single-particle states up to the Fermi energy are occupied by one and only one nucleon. In an excited state, one or more of the particles occupy states above the Fermi energy, leaving the same number of holes below the Fermi energy. Each distinct arrangement of the particles and holes (taking into account indistinguishability and the exclusion principle) defines a particle-hole configuration. Energy is assumed to be conserved at all times, so that only the subset of the particle-hole configurations with the same excitation energy E^* needs to be considered in a given reaction. The exciton number of a configuration is defined as the sum of the numbers of active particles and holes. An exciton class is defined as the set of configurations with the same numbers of active particles and holes and, thus, the same exciton number. To be in agreement with the description above of the particle-hole nature of an excited state, we would want to denote the exciton configurations as being 2p-2h (two-particle-two-hole), 3p-3h, and so on. However, in the exciton model, the hole of the initial 1p-1h state of the nucleon-target composite system is assumed to be fixed at the Fermi energy. It is not considered an active degree of freedom and is not allowed to participate in the reaction. The usual exciton model nomenclature thus refers to 2p-1h, 3p-2h, and similar configurations. The HMS model makes a similar assumption when it initiates a reaction through the production of a 2p-1h configuration.

The two models thus assume a nucleon-induced reaction to be initiated by the fusion of the projectile nucleon and the target to form a 2p-1h configuration. The system can then proceed to 3p-2h and more complicated np-(n-1)hconfigurations through two-body transitions, or it can emit a nucleon, if one of them has sufficient energy. Pre-equilibrium nucleon emission is simply emission that occurs before the particle and hole degrees of freedom excited in the reaction have attained equilibrium. Since the excitation energy is shared by few degrees of freedom in the initial stage of the reaction, pre-equilibrium emission is characteristically of higher energy than that expected of equilibrium.

Because of the two-body nature assumed for the internal nuclear transitions, these can excite another particle-hole pair and increasing the exciton number by two, scatter two particles, two holes, or a particle and a hole and leave the exciton number the same or annihilate a particle-hole pair and reduce the exciton number by 2. The transitions annihilating a particle-hole pair are often neglected in pre-equilibrium model calculations. Known as the never-come-back approximation, this usually furnishes a reasonable approximation to emission from the configurations of low exciton number, the ones most important for pre-equilibrium emission. It is less reliable in light nuclei and at low excitation energy and should certainly not be expected to provide reasonable results beyond the first few stages of a reaction. The transitions that do not alter the exciton number mix the configurations within each exciton class. These enter into neither the HMS nor the exciton models, although for very different reasons.

The HMS model. As shown by Bisplinghoff [27], the hybrid model [8] neglects all transitions between configurations of the same exciton class. This is also true of its successor, the hybrid Monte Carlo simulation (HMS) model [28,29]. The HMS model describes the reaction cascade in terms of a sequence of 2p-1h excitations created by the incident nucleon or by one of the subsequent particles and of 1p-2h excitations generated by the holes. The emission and transition rates are calculated using the inverse absorption cross section and a medium-corrected nucleon-nucleon scattering cross section, respectively. Since no mixing is taken into account, the excitations are well-defined configurations that are altered only when a particle or hole participates in a subsequent collison or when a particle is emitted. The HMS uses only 2p-1h, 1p-1h, and 1p-2h state densities, since these densities can be shown to be consistent with the kinematics of a nucleon-nucleon collision or emission, in the absence of mixing [10,27]. The HMS model also makes use of the never-come-back approximation and so it must be truncated in some manner. This is done by removing from the calculation any particles or holes whose excitation energies are insufficient for particle emission. Their accumulated excitation energy is subsequently used to calculate the equilibrated compound nucleus contribution to the spectrum.

The HMS model, like the hybrid model, calculates inclusive emission spectra. We take this to be a consequence of the manner in which the calculations are performed rather than an intrinsic property of the model. At each step of the cascade, the HMS model chooses between emission and creation of a particle-hole pair based only on the emission and transition rates of the single-particle state occupied by an arbitrary particle. The model does not compare the relative emission/transition rates of different particles and holes. If it were do so, that is, if it were to base its choices on the comparison between the partial widths for emission or transition of all existing particles and holes, the HMS model could calculate exclusive spectra. Since the model does not make such a comparison, the inclusive spectra that it produces are not necessarily the same as those obtained in an exclusive emission model. A drawback of an exclusive emission calculation, however, is that it is a much more time-consuming process.

The exciton model. The exciton model assumes that the configurations of an exciton class are equally populated at each stage of the reaction cascade. Transition and emission rates based on state and transition densities for the exciton classes can then be used [11,14,26,41,42], which greatly simplifies numerical calculations. As in the hybrid and HMS models, emission rates are calculated using the inverse absorption cross section. Transition rates are calculated using either a medium-corrected nucleon-nucleon cross section [13,15,26] or a parametrization of the average mean-squared two-body interaction matrix element [12,25,26]. Due to the assumption of equal occupations within each class, transitions between configurations within a class can have no effect and for this

reason play no role in the exciton model. The emission and transition rates represent averages over the configurations in each exciton class that, by taking into account all the active degrees of freedom of each of the configurations, furnish exclusive emission spectra.

The exciton model obtains its simplicity from the assumption of equal occupation of the configurations in each exciton class. There are two manners in which this could be achieved. Either the internal transitions that change the exciton number yield (nearly) equal occupation probabilities at each stage, or the transitions within each class strongly mix the configurations before emission or transition to another class occurs. The exciton model possesses a means of checking its conceptual consistency with the second of these. For the configuration mixing in each exciton class to be so strong as to be (nearly) complete, the transition rate between configurations of a given exciton class must necessarily be much larger than the transition rates between classes. In the exciton model, it is possible to calculate the transition rate between configurations of the same class, $\lambda_0(n)$, *n* being the exciton number, just as easily as the rates of transitions that increase and decrease the exciton number by two, $\lambda_{+}(n)$, and $\lambda_{-}(n)$, respectively. [As mentioned above, due to the equilibrium hypothesis, the transition rate $\lambda_0(n)$ does not appear in the exciton master equation governing the evolution of the system.]

In Fig. 1, we display the transition rates for a 40-nucleon system as a function of the number of holes h, at excitation energies of 25 and 100 MeV. The transition rates at 25 MeV extend to h = 10, while those at 100 MeV extend to h = 18. For a given exciton number n, the rate for transitions that increase the exciton number $\lambda_+(n)$ increases with excitation energy and the rate for transitions that decrease the exciton number $\lambda_-(n)$ decreases with energy, while the transition rate between configurations of the same exciton class $\lambda_0(n)$ remains almost constant. At both excitation energies, we see that the transition rate $\lambda_0(n)$ is smaller than the transition rate $\lambda_+(n)$ at low exciton number. As the excitation energy increases,



FIG. 1. (Color online) Exciton model transition rates $\lambda_+(n), \lambda_0(n)$, and $\lambda_-(n)$ of a 40-nucleon system as a function of the number of holes *h*, at excitation energies of 25 (those extending to h = 10) and 100 MeV (those extending to h = 18).

the number of stages at which $\lambda_0(n) \leq \lambda_+(n)$ also increases. Thus we do not expect internal configuration mixing to provide the equal occupation probabilities of the exciton model in the initial stage of the reaction cascade. We also expect this initial stage of the cascade to become longer as the excitation energy increases. We note that at the equilibrium exciton number, where $\lambda_+(n) = \lambda_-(n)$, the transition rate $\lambda_0(n)$ is at most about a factor of 2 greater than the others, making the hypothesis of class equilibrium due to configuration mixing somewhat dubious even there.

It is still possible to establish equilibrium between transitions that increase the exciton number and those that decrease it, even with no internal configuration mixing at all. Evolution to an equilibrated compound nucleus will occur whenever emission rates are much smaller than the internal transition rates, whether the latter mix the configurations in each class or not. The occurrence of equal probabilities within each exciton class, however, does not appear to be consistent with the exciton model estimate of configuration mixing.

In the following, we develop a unified model that permits us to simulate varying degrees of configuration mixing and use the model to examine its effects in more detail.

III. A UNIFIED SEMICLASSICAL PRE-EQUILIBRIUM MODEL

We take the single-particle spectrum of the model to be uniformly spaced, with the spacing between states, ΔE , determined so that the most deeply bound nucleon of the A + 1 target-nucleon system is bound by 45 MeV while the projectile nucleon, if it were in its fundamental state at the Fermi energy, would be bound by a separation energy *B* of about 8 MeV. The initial configuration of the system is taken to be a 1p-1h one, with the hole at the Fermi energy and the particle (the projectile nucleon) occupying the single-particle state closest in excitation energy E^* to $E_n + B$ MeV, where E_n is the incident center-of-mass energy. We do not distinguish between neutrons and protons.

We treat each particle-hole configuration explicitly. Thus, we consider the 1p-1h configuration consisting of a particle of energy ε_{p1} and a hole of energy ε_{h1} to be distinct from the 1p-1h configuration consisting of a particle of energy ε_{p2} and a hole of energy ε_{h2} if $p1 \neq p2$ or $h1 \neq h2$. We label each particle-hole configuration by a letter from the beginning of the alphabet a, b, c, \ldots as well as a by class label l, m, n, \ldots denoting the total number of particles and holes. The class label is actually redundant, being completely determined by the configuration, but it is useful when considering the exciton-model limit. We denote the occupation probability of a typical configuration as P_{na} .

Master equation. The configuration occupation probabilities are governed by a master equation,

$$\hbar \frac{dP_{na}}{dt} = \sum_{mb} \Lambda_{na,mb} P_{mb} - \Gamma_{na} P_{na}, \qquad (1)$$

where the total decay width of the configuration na is given in terms of the partial transition widths $\Lambda_{lc,na}$ and partial emission

widths $\Gamma_{e,na}$ by

$$\Gamma_{na} = \sum_{lc} \Lambda_{lc,na} + \sum_{e} \Gamma_{e,na} \,. \tag{2}$$

The rate of emission of particles of energy *e* is given by

$$\frac{dS_e}{dt} = \frac{1}{\hbar} \sum_{na} \Gamma_{e,na} P_{na} \,. \tag{3}$$

Emission. We estimate emission using the usual Weisskopf expression, which can be determined from reciprocity. We take the partial width for nucleon emission from the configuration na in an interval ΔE of emission energy e to be

$$\Gamma_{e,na} = \frac{g_s \mu}{\pi^2 \hbar^2} e \sigma_{abs}(e) \frac{1}{r} \Delta E, \qquad (4)$$

if the configuration contains a particle of energy e + B, where *B* is the separation energy, and as zero otherwise. Here, $g_s = 2$ is the nucleon spin multiplicity, μ is the reduced mass, and $\sigma_{abs}(e)$ is the absorption cross section, which we approximate geometrically as $\sigma_{abs}(e) = \pi R^2$. The total emission width of a configuration is the sum of the partial widths of each of the particles that can be emitted.

Because we use a uniformly spaced spectrum of singleparticle states, the value of our single-particle state density, $g \approx$ $A/37 \,\mathrm{MeV^{-1}}$, is much smaller than the phenomenological one, $g \approx A/13$ MeV⁻¹. A possible explanation of the difference is given in Appendix A, where we show that the singleparticle state density of a three-dimensional (3-D) harmonic oscillator is a factor of 3 larger, at the Fermi energy, than the single-particle density of the uniformly spaced states of a one-dimensional (1-D) harmonic oscillator. Exciton model calculations are often performed using state and transition densities based on a uniformly spaced spectrum together with the constant value of the single-particle state density corresponding to the value of an energy-dependent density evaluated at the Fermi energy. We cannot do this here, however, since we treat each configuration distinctly. We can obtain similar results by modifying the emission and transition rates appropriately, as shown in Appendix A. The factor $r \approx 3$, included in the partial emission width above, modifies it so as to simulate the effect of the larger phenomenological density of single-particle states.

Transitions. We consider transitions induced by energyconserving two-body collisions and denote the partial width for the transition from mb to na as $\Lambda_{na,mb}$. We assume microscopic reversibility, so that $\Lambda_{na,mb} = \Lambda_{mb,na}$. Since the transitions are due to two-body interactions, the nonzero partial transition widths will increase the number of particles and holes by 2, $\Lambda_{n+2a,nb}$, leave it the same, $\Lambda_{na,nb}$, or decrease it by 2, $\Lambda_{n-2a,nb}$. If the transition from a configuration mb to a configuration na is possible, the two-body collision inducing it is unique. The partial width of any transition can thus be associated with the squared matrix element of the corresponding two-body interaction. If we assume that all two-body collisions are equally likely, that is, that all squared two-body matrix elements are equal, we can then associate a single value to all nonzero partial transition widths. We take this to be the value associated with the average squared matrix element of the exciton model [12,25,26], which we

approximate as

$$\Lambda_{na,mb} = 2\pi |M|^2$$

$$= \begin{cases} 2\pi \frac{f_0}{A^3 E^*} & f_0 \approx 1350 \text{ MeV, when } mb \to na, \\ 0 & \text{otherwise,} \end{cases} (5)$$

where the constant f_0 was adjusted using the simple form of Ref. [12] so as to best reproduce the expression given in Eq. (29) of Ref. [26].

To simulate the effect of a larger single-particle state density, we multiply the transition rates that increase the number of particles and holes by a factor r^3 , the transition rates that do not change the number of particles and holes by a factor r^2 , and the transition rates that decrease the number of particles and holes by a factor r, where $r \approx 3$ (see Appendix A). We emphasize that were it not for the factor r, the partial transition widths would be the same for all allowed transitions. The factor r was inserted to simulate the effect on the transition densities of the difference between the actual single-particle state density of our calculations and that expected phenomenologically. In the following, we call this the natural model. The values of the partial transition widths given here would furnish the transition rates of the usual exciton model, if they were summed over all transitions between the various exciton classes.

No mixing and the HMS model. By varying the transition rates among the different classes of states, we can study the effects of various degrees of configuration mixing. By taking $\Lambda_{na,nb} \rightarrow 0$, we eliminate the internal mixing of the configurations in each exciton class. The lack of internal mixing is the basic distinguishing characteristic of the hybrid and HMS models. If we were to make the never-come-back approximation as well, $\Lambda_{n-2a,nb} \rightarrow 0$, which we will not do, we would obtain a model with fundamental properties identical to those of the HMS model of Ref. [28]. In addition, as formulated here in terms of a master equation, the no-mixing limit of the model provides exclusive spectra rather than the inclusive ones calculated in the HMS model.

Complete mixing and the exciton model. When the partial widths for transitions within an exciton class are much larger than those between classes,

$$\Lambda_{na,nb} \gg \Lambda_{na,mb}, \Lambda_{mb,na} \qquad m = n \pm 2, \qquad (6)$$

the configurations within each exciton class tend to equilibrium between the occurrence of transitions between exciton classes. That is, the occupation probabilities tend to

$$P_{na} \to \frac{1}{N_n} P_n,$$
 (7)

where N_n is the total number of configurations of excitation energy E^* in exciton class n, and $P_n = \sum_a P_{na}$ is the total occupation probability of the class. If equilibrium among configurations in each class is indeed reached, we can write the master equation as

$$\hbar \frac{1}{N_n} \frac{dP_n}{dt} = \sum_{mb} \Lambda_{na,mb} \frac{1}{N_m} P_m - \Gamma_{na} \frac{1}{N_n} P_n, \qquad (8)$$

which, after summing over all configurations in each exciton class, can be rewritten as

$$\hbar \frac{dP_n}{dt} = \sum_m \Lambda_{n,m} P_m - \Gamma_n P_n, \qquad (9)$$

with

$$\Lambda_{n,m} = \sum_{ab} \Lambda_{na,mb} \frac{1}{N_m} \quad \text{and} \quad \Gamma_n = \sum_m \Lambda_{m,n} + \sum_e \Gamma_{e,n},$$
(10)

where

$$\Gamma_{e,n} = \sum_{a} \Gamma_{e,na} \frac{1}{N_n} \,. \tag{11}$$

The rate of emission of particles of energy e can now be written as

$$\frac{dS_e}{dt} = \frac{1}{\hbar} \sum_n \Gamma_{e,n} P_n \,. \tag{12}$$

In this limit, the model reduces to the usual exciton model, in which system evolution and emission rates depend only on the populations of the exciton classes and not those of the individual configurations. Note that the contribution from transitions within a class, $\Lambda_{n,n} P_n$, exactly cancels the same contribution in $\Gamma_n P_n$, so that these transitions no longer contribute to the evolution of the system.

IV. NUMERICAL RESULTS

In the unified model, the number of particle-hole configurations in a typical calculation is usually extremely large. In the case of a nucleon incident on ¹⁶O at 20 MeV, about 600 configurations come into play and, thus, about 600 coupled equations would be required, while about 43 000 configurations are involved at 100 MeV. In the case of a nucleon incident on ⁵⁶Fe at 100 MeV, the number of configurations is on the order of 130 million. Direct solution of the master equation is simply not viable in general. We use instead a Monte Carlo simulation method to obtain emission spectra (see Appendix B). This has the advantage of being easily parallelizable, which permits fairly rapid calculations of the model on a cluster of personal computers (PC's). The calculations presented here were, for the most part, performed using eight PC's of the BELIEVe II cluster at the Instituto de Estudos Avançados-CTA.

In the following, we denote as natural model simulations those in which the partial widths for internal transitions are identical but for the factor r simulating the effects of a larger single-particle state density. We denote as no-mixing calculations those in which internal mixing has been eliminated by taking $\Lambda_{na,nb} \rightarrow 0$. We denote as complete-mixing calculations those simulations in which the transitions between configurations of the same exciton class have been taken to be a factor of 1000 larger than those used in the natural model. None of the unified model simulations use the never-come-back approximation.

We also perform exciton model calculations using the class transition and emission rates obtained from the sums over

configurations given in Eqs. (10) and (11). The calculations use the exact sums over the configurations, rather than the approximate expressions given in Appendix A, and we use standard coupled linear equation methods to solve the timeintegrated master equation [Eq. 48 of Appendix B].

In the simulations, each Monte Carlo cascade was initiated from a 1p-1h configuration in which the excitation energy is carried by the particle, and the hole is at the Fermi surface. This hole is normally maintained fixed at the Fermi surface when pre-equilibrium exciton densities and transition rates are calculated, resulting in np-(n-1)h hole quantities. In contrast, statistical models of the equilibrated compound nucleus take all np-nh densities into account, which would imply that the hole at the Fermi surface has been allowed to equilibrate with the other nuclear degrees of freedom. To take both possibilities into consideration, we performed simulations of the complete-mixing model and standard exciton model calculations for the two cases: with the hole fixed and with it free to interact. We denote the fixed-hole simulations as Mix1 and the free-hole simulations as Mix0. To avoid the strong 1p-1h component that would be excited in the completemixing model if the hole were free in the initial interaction (due to the factor of 1000 multiplying the intraclass transition rate), we also fix the hole at the Fermi surface for the initial interaction in the Mix0 simulations. Thus both completemixing simulations, Mix0 and Mix1, start with the same 2p-1h-1fixed hole distribution. In the no-mixing and natural model simulations, the hole is free to interact at all stages of the reaction. In all cases, to ensure formation of a composite system, emission is not permitted in the first interaction. Since we consider all particles and holes as active degrees of freedom, except in the cases of the Mix1 simulations and the corresponding exciton model calculations, we label the configuration classes as *np-nh* ones in the following. In the cases of the Mix1 simulations and corresponding exciton model calculations, of course, one of the holes is fixed at the Fermi surface.

We performed Monte Carlo simulations to obtain the emission spectra for a nucleon incident on systems of 16, 40, 56, and 90 nucleons in an incident energy range from 8 to 200 MeV. The Monte Carlo calculations were truncated according to the quantity under study. For example, simulations run with the intent of obtaining the emission spectrum from the np-nh class were truncated after emission or a transition to the (n + 1)p-(n + 1)h class, as described in more detail below. Simulations run with the intent of obtaining the emission spectrum of the *n*th nucleon were truncated after the emission of n nucleons. To calculate total emission spectra, the simulations were allowed to run until particle emission was no longer possible. To construct each of the emission spectra, we followed 10^6 cascades. We found the variation with incident energy of the spectra to be similar for the four systems. Here, we present our results for the 40-nucleon system, since it is the heaviest system for which our standard exciton calculations are also more or less complete. Our routine for performing the explicit configuration sums for the standard exciton model calculations was simply too time consuming for the heavier systems except at the lowest energies.



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FIG. 2. (Color online) Spectra of the first nucleon emitted from the 2p-2h, 3p-3h, 4p-4h, and all stages of a nucleon + 40-nucleon system at an incident energy of 50 MeV. The Monte Carlo calculations are represented by histograms as labeled in the figure and discussed in the text. The thin lines correspond to standard exciton model calculations.

In Fig. 2, we show spectra of the first emitted nucleon from the nucleon +40-nucleon system at an incident center-of-mass-energy of 50 MeV at several stages of the reaction. The Monte Carlo simulations are shown as histograms while the exciton model calculations are displayed as thin lines. The Monte Carlo spectra labeled np-nh correspond to emission from the np-nh stage of the reaction before the (n + 1)p(n + 1)h stage is reached. That is, the spectra labeled 2p-2h were obtained by stopping the Monte Carlo calculations after one emission or when a transition to a 3p-3h configuration occurred. Since no emission is allowed from the initial 1p-1h configuration, any emission in these cases necessarily occurred at the 2p-2h stage of the reaction. The 3p-3h and 4p-4h emission spectra are obtained by stopping the Monte Carlo simulations after one emission or when a transition took place to a 4p-4h or 5p-5h configuration, respectively, and then subtracting the spectrum corresponding to the preceding stage. The never-come-back hypothesis was used to calculate the standard exciton model spectra shown with these curves, since this hypothesis is more consistent conceptually with the truncation of the cascade used to obtain the Monte Carlo spectra than a calculation without it. The spectra corresponding to emission of the first nucleon from any stage of the composite system are also shown. In these cases, the never-come-back hypothesis was not used to obtain the standard exciton model spectra. We note the excellent agreement between the complete-mixing and standard exciton model spectra at each stage of the reaction, in both the fixed-hole (Mix1) and free-hole (Mix0) cases. The no-mixing and natural model simulations are also in very close agreement with one another. The fixed-hole complete-mixing spectra are substantially harder than the no-mixing and natural model ones at each of the initial stages and in the overall onenucleon emission spectrum. The free-hole complete-mixing spectrum, on the other hand, is softer in the initial stage of the reaction but is harder than the no-mixing and natural models by the 4p-4h stage. However, it is the first stage of the reaction that dominates the overall one-nucleon emission spectra, with the fixed-hole complete-mixing spectra being harder than the no-mixing and natural ones, which are almost identical, and the free-hole complete-mixing spectra being the softest.

The hardness of the fixed-hole complete-mixing spectra relative to the others can be understood in terms of the energy dependence of the partial emission widths and the effects of the transitions within each exciton class. The partial emission width of Eq. (4) increases monotonically (in our case, linearly) with the energy of the emitted nucleon. A nucleon in a low-positive-energy single-particle state thus has a smaller probability of being emitted than one in a higher-energy state. In a no-mixing simulation, a nucleon initially in a low-positiveenergy single-particle state may either interact to annihilate a hole state, interact to create yet another particle-hole pair, or be emitted. Although the first of the two internal transitions could result in a more energetic nucleon, the probability of such an annihilation is extremely low in the early stages of a reaction. In a complete-mixing simulation, the probability of transitions within each exciton class is high. In the fixed-hole complete-mixing model, the result is that nucleons initially in low-positive-energy single-particle states tend to be promoted to higher-energy ones before being emitted. Just the opposite occurs in the free-hole complete-mixing model, where the energy dependence of the particle-hole density of states including the additional degree of freedom dominates the energy dependence of the partial emission width, favoring emission from the more numerous states in which the particle energy is lower. The close agreement between the no-mixing and natural model spectra leads one to conclude that the intraclass transitions of the natural model are relatively ineffective.

In Fig. 3, we show spectra of the first emitted nucleon from the nucleon + 40-nucleon system at an incident center-of-mass energy of 100 MeV at the same stages of the reaction. The Monte Carlo simulations are again shown as histograms, while



FIG. 3. (Color online) Same as Fig. 2, but at an incident energy of 100 MeV.

standard exciton model calculations are displayed as thin lines. The complete-mixing spectra and the exciton model spectra are again in excellent agreement, as are the no-mixing and natural model simulations. The fixed-hole complete-mixing and exciton model spectra, although still harder than the the no-mixing and natural model ones, appear to be in closer agreement with them in the initial stage of the reaction. The free-hole complete-mixing and exciton model spectra, in contrast, are now much softer than the others at the initial stage of the reaction but follow the no-mixing and natural model spectra partially at the 4p-4h stage. The differences in the total one-nucleon emission spectra are again basically those of the initial stage of the reaction, with the free-hole complete-mixing and exciton model spectra being the softest and the fixed-hole complete-mixing and exciton model spectra being harder than the no-mixing and natural ones, which are again almost identical.

The Monte Carlo simulations can be easily extended beyond the first emission. This is done by moving the Fermi energy down one state after each emission occurs, so as to be in accord with the nucleon number of the residual nucleus, and continuing the calculation. In the case of the fixed-hole complete-mixing model simulations, the fixed hole becomes an empty particle state after particle emission, so that all degrees of freedom participate freely in the subsequent stages of the reaction. In all cases, the cascade of transitions and emissions may be continued until the remaining excitation energy is insufficient for further particle emission. We did not extend the standard exciton model calculations beyond the first emission, although this can be done [26].

In Fig. 4, we show the inclusive nucleon emission spectra from the nucleon + 40-nucleon system at the incident centerof-mass energies of 25, 50, 100, and 200 MeV. The no-mixing and natural model spectra are again in excellent agreement at all incident energies. The free-hole complete-mixing model produces spectra which are consistently softer than the others. The fixed-hole complete-mixing spectra, harder than the others at lower incident energies, seem to reach ever better agreement with the no-mixing and natural model spectra at higher incident energies. This trend is quite remarkable. We would expect that the no-mixing and natural model simulations might attain the partial equilibrium intrinsic to the complete-mixing model at lower energies, where emission is slower compared to the internal transitions, rather than at higher ones. Yet it is at lower energies that the fixed-hole complete-mixing emission spectra are most visibly different from the no-mixing and natural model ones.

A look at other characteristics of the reaction reveals that only the model spectra become similar at higher energies. In Fig. 5, we show the average nucleon multiplicity, that is, the average number of emitted nucleons, as a function of incident energy for the different simulations. The vertical lines show the standard deviation of the natural model multiplicity, the standard deviations of the other models being similar. As with the spectra, we find the no-mixing and natural model simulations to yield almost identical results. Surprisingly, we find that free-hole complete-mixing simulations also furnish multiplicities very close to the no-mixing and natural ones, in spite of their consistently softer spectra. The multiplicities of the fixed-hole complete-mixing simulations, on the other hand, become increasingly smaller than the others as the incident energy grows. At 200 MeV, the fixed-hole complete-mixing simulations emit, on the average, almost one nucleon less than the others do.

An interesting detail of the simulations is the flattening of the average multiplicity curve and a decrease in its standard deviation below the threshold for three-nucleon emission. With only two possibilities, emission of either one or two nucleons, and the constraint of probability conservation, the average multiplicity in this case is given by $\langle n \rangle = 1 + P(2)$, where P(2) is the probability of emitting two nucleons. As P(2)increases with energy, the system tends toward saturation at multiplicity 2. Since this effect appears in the simulations of all systems we have studied, it might well be observable



in physical systems, in particular, in heavy nuclei, where charged-particle emission is inhibited. Above the three-particle emission threshold, the average multiplicity and its standard deviation grow monotonically in all of the simulations.

The multiplicity distribution P(n) gives a better overall picture of the reaction than the average multiplicity alone. The distribution is shown in Fig. 6 for the incident center-of-mass energies of 25, 50, 100, and 200 MeV. The distributions become quite broad as the energy increases, even broader than the standard deviation of the average multiplicity might suggest. At 200 MeV, multiplicities from 1 to 17 are possible, and those from 2 to 14 occur at least a few percent of the time. The lower average multiplicity of the fixed-hole complete-mixing simulations is also clearly reflected in the shift of their distributions to lower values at all energies.



The relative disposition of the distributions at low multiplic-

The distributions at high multiplicity reflect the effects of the configuration mixing within each of the exciton classes. From Fig. 6, it is clear that high multiplicity reactions are less probable in the complete-mixing models than in the



FIG. 5. (Color online) Average nucleon emission multiplicity as a function of the incident energy. Thin vertical lines represent the standard deviation of the multiplicity of the natural model.



FIG. 6. (Color online) Nucleon emission multiplicity distributions of a nucleon + 40-nucleon system at incident energies of 25, 50, 100, and 200 MeV.

FIG. 4. (Color online) Inclusive nucleon emission spectra for a nucleon + 40-nucleon system at incident energies of 25, 50, 100, and 200 MeV.



FIG. 7. (Color online) Same as Fig. 2, but for various values of the intraclass transition strength.

others, with high multiplicity the least probable in the fixedhole complete-mixing model. High multiplicity requires the emission of low-energy nucleons. As discussed above, the mobility of nucleons in the complete-mixing models, due to the large intraclass transition rates, enhances the emission of high-energy nucleons in the fixed-hole case and suppresses it in the free-hole case. The nucleon mobility suppresses the emission of low-energy nucleons in both cases, since both the partial emission width and the density of particle-hole states disfavor states containing these nucleons. The probability of high multiplicity is slightly larger in the free-hole model because the energy is shared by more degrees of freedom, thus decreasing the average energy of each of the holes and particles. The differences between the natural model distributions and the no-mixing one at high multiplicity can be associated with the same effects of the intraclass transitions. The effects are much smaller in this case, but still clearly visible.

In summary, we have found that the no-mixing and natural model emission spectra and multiplicity distributions are almost identical. The only significant difference found between the two is that of the multiplicity distributions at high energy, where the internal mixing makes high multiplicity slightly less probable in the natural model. The complete-mixing results are identical to the corresponding standard exciton model results, but the two versions of these models, in which a hole is fixed or not, are very different from one another. The fixed-hole complete-mixing model furnishes spectra close to those of the no-mixing and natural models at high energies, but underestimates the average multiplicity there, when compared to the other two. The free-hole complete-mixing model yields softer spectra than the other models at all incident energies.

There is still an important question that should be asked. Is the factor of 1000 multiplying intraclass transitions really necessary to provide the equilibrium presumed in the complete-mixing model? Might 100 or even 10 be enough? A value smaller than 1000 would certainly be more natural.

We reply with Fig. 7, where we show spectra of the first emitted nucleon from the nucleon + 40-nucleon system at an incident center-of-mass energy of 50 MeV at several stages of the reaction for values of the factor multiplying intraclass transitions of 10, 100, and 1000. Recall that the natural model uses a factor of 1, but does not fix the hole at the Fermi energy. The Monte Carlo simulations are shown as histograms while the fixed-hole standard exciton model calculations are displayed as thin lines. The fixed-hole simulations using an intraclass factor of 10 fall closer to the no-mixing and natural model spectra than to the standard exciton model one. The simulations using a factor of 100 come closer but are still very distinguishable from the standard exciton model calculations, which lie atop the simulations using a factor of 1000. The free-hole simulations (not shown) fall in an almost symmetrical fashion on the other side of the no-mixing and natural model calculations, tending toward the corresponding standard exciton model calculation as the multiplicative factor tends to 1000. We conclude that a factor on the order of 1000 is indeed necessary to provide class equilibrium in both complete-mixing simulations.

V. CONCLUSIONS

We have developed a unified model of semiclassical nucleon-induced pre-equilibrium reactions and used it to simulate the cases of no intraclass mixing and complete intraclass mixing, as well as an intermediate case that we call the natural model. We defined the natural model as that in which the transitions between configurations of the same exciton class are of the same intensity as those that change the exciton class. We simulated the no-mixing model by eliminating the transitions among configurations within each exciton class. To simulate the complete-mixing model, we found it necessary to make the transitions among configurations of an exciton class a thousand times greater than those of the natural model. We considered two variations of the complete-mixing model: the usual one, in which a hole is fixed at the Fermi surface, and one in which all of the degrees of freedom are free to interact.

What can we conclude? First, we have seen that the no-mixing and natural model emission spectra and multiplicity distributions are almost identical, with the only significant difference between the two being the slightly higher probability of high multiplicity in the no-mixing model at high incident energies. This tells us that the internal configuration mixing of the natural model is little more effective than no mixing at all. Second, we have seen that the complete-mixing results are identical to the standard exciton model results but are quite different from the those of the no-mixing and natural models. This tells us two things: the complete-mixing simulations with transitions a thousand times stronger than the natural ones do indeed attain the class equilibrium presumed in the standard exciton model, and the no-mixing and natural model simulations describe emission from systems that do not attain this equilibrium. Furthermore, the large differences between the no-mixing and complete-mixing results tell us that the transitions between exciton classes do not result in equal occupation probabilities. If they did, we would see no difference between the emission spectra of the two limiting models. Thus, complete intraclass mixing is the only means to obtain equal occupation of the configurations within an exciton class. Yet, it is difficult to imagine a mechanism that would furnish intraclass matrix elements a thousand times larger than the interclass ones, as is needed to obtain complete intraclass mixing. We also find the fixed-hole complete-mixing model to suffer from the additional inconsistency of fixing a hole at the Fermi surface while allowing all other degrees of freedom to interact strongly. In summary, the complete-mixing models require that one subset of the transitions be, anomalously, a thousand times stronger than the others and then offer us a choice between a fixed-hole version that is conceptually inconsistent and a free-hole version that cannot possibly describe the experimental data. We see no alternative but to reject both. We conclude that the no-mixing and natural models provide the more consistent description of pre-equilibrium reactions and that the intraclass equilibrium of the completemixing and exciton models is not attained in the early stages of these reactions.

The results obtained here are also pertinent to quantummechanical models of pre-equilibrium reactions. In these, the interaction plays a dual role, being responsible for the transitions among configurations as well as determining the manner in which statistical hypotheses may be invoked to eliminate quantum interference. The statistical hypotheses of these models have been classified into two types: leadingparticle statistics, in which the matrix elements of the states excited by the incident nucleon are represented by a random variable, and residual-system statistics, in which the configuration mixing introduces the random character [21,22]. We can say nothing about leading-particle statistics here, since we do not distinguish the leading particle from the others after the first interaction in our simple model. However, our conclusions tell us that residual-system statistics, such as those used in most multistep compound models [16,17,19] and in the multistep direct model of Tamura, Udagawa, and

Lenske [18], are not justified if they are based on the mixing of particle-hole configurations. Residual-system statistics might still be justifiable if they were to be based on some more general set of states, such as nested doorway ones [43–45], although the microscopic nature of such a set of states is not clear to us. We note that the multistep direct model of Nishioka, Weidenmüller, and Yoshida [20] also uses residual-system statistics, but it confines them to the final states of the system, where they are justifiable for any set of states.

Although we have found them wanting, the hypotheses of the exciton model result in expressions that are exceedingly easy and rapid to calculate. When comparing with experimental data, adjustment of the model's average matrix element is often enough to produce an excellent fit. The exciton model will thus certainly be used for some time to come in phenomenological applications. However, we believe it is time for more conceptually consistent models to begin to take its place. As our next step in this direction, we plan to develop a more physical version of the no-mixing model, one that would have much in common with an exclusive version of the HMS model.

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APPENDIX A: EXCITON MODEL DENSITIES

This Appendix briefly describes the densities of states and of transitions used in the standard exciton model. None of these densities are used in the calculations presented. They are discussed here in order to justify the use of the factor r, which converts the emission and transition factors of the unified model to the effective phenomenological ones.

1. Single-particle densities of states

For the 1-D harmonic oscillator, we can enumerate the states as

$$E_n = \hbar \omega \left(n - \frac{1}{2} \right)$$
 $n = 1, 2, 3, \dots,$ (A1)

where n is the principal quantum number. We rewrite this as

$$n_1(E) = \frac{E}{\hbar\omega} + \frac{1}{2},\tag{A2}$$

where $n_1(E)$ is the number of states with energy less than or equal to *E*. At the Fermi energy, taking into account the spin-isospin degeneracy of a $Z \approx N$ system, we then have for the single-particle density of states g_1

$$4n_1(E_F) = A$$
 and $g_1 = 4 \left. \frac{dn_1}{dE} \right|_{E_F} \approx \frac{A}{E_F}.$ (A3)

In the case of the 3-D harmonic oscillator, we can enumerate the levels as

$$E_{nl} = \hbar \omega \left(2n + l - \frac{1}{2} \right) \qquad \begin{array}{l} n = 1, 2, 3, \dots, \\ l = 0, 1, 2, \dots, \end{array}$$
(A4)

where n is the principal quantum number and l is the angular momentum.

It is a simple matter to invert this and write

$$n(E,l) = \frac{1}{2} \left(\frac{E}{\hbar\omega} + \frac{1}{2} - l \right) \qquad l < \frac{E}{\hbar\omega} + \frac{1}{2}, \qquad (A5)$$

where n(E, l) is the number of levels with energy less than or equal to *E* and angular momentum *l*. We treat n(E, l) as a continuous quantity, rewriting it as

$$n(E, l) = \frac{1}{2}(l_m - l) \qquad l < l_m,$$
 (A6)

with

$$l_m = \frac{E}{\hbar\omega} + \frac{1}{2}.$$
 (A7)

We can calculate now the total number of levels with energy less than or equal to E, as

$$N_{\rm lev}(E) = \int_0^{l_m} n(E, l) dl = \frac{l_m^2}{4}.$$
 (A8)

The corresponding density of single-particle levels is then

$$\rho_{\rm lev}(E) = \frac{d}{dE} N_{\rm lev}(E) = \frac{l_m}{2} \frac{dl_m}{dE}.$$
 (A9)

We can also calculate the total number of single-particle states with energy less than or equal to E as

$$N_s(E) = \int_0^{l_m} (2l+1)n(E,l) \, dl \approx \int_0^{l_m} 2ln(E,l) \, dl = \frac{l_m^3}{6},$$
(A10)

and the corresponding density of states

$$\rho_s(E) = \frac{d}{dE} N_s(E) = \frac{l_m^2}{2} \frac{dl_m}{dE}.$$
 (A11)

Taking into account the spin-isospin degeneracy of the nuclear states and assuming a spin-saturated nucleus with $N \approx Z$, we can write the total number of states with energy less than or equal to *E* as

$$N_{\text{tot}}(E) \approx 4N_s(E) = \frac{2}{3}l_m^3.$$
 (A12)

At the Fermi energy, we have

$$N_{\rm tot}(E_F) = A. \tag{A13}$$

The 3-D density of states at the Fermi energy g_3 is then

$$g_3 = \rho_{\text{tot}}(E_F) = 2l_m^2 \frac{dl_m}{dE}\Big|_{E_F} = 3A \frac{1}{l_m} \frac{dl_m}{dE}\Big|_{E_F}.$$
 (A14)

From the definition of l_m , we have

$$\frac{1}{l_m}\frac{dl_m}{dE} \approx \frac{1}{E}$$
 and $g_3 \approx 3\frac{A}{E_F}$. (A15)

We take $E_F \approx 37$ MeV in our calculations, so that we have $g_3 \approx 3g_1 \approx A/13$ MeV⁻¹.

In the following, we rewrite the exciton transition densities and partial emission widths in terms of the number of states in bins of size $\Delta E = 1/g_1$, in order to justify the factors of $r = g_3/g_1 \approx 3$ in the partial widths of the unified model.

2. Density of states

We assume that the excitation energy can be written as $E^* = N^* \Delta E$ and the Fermi energy as $E_F = N_F \Delta E$.

The particle-hole state density in a uniform-spacing model can be well approximated by [14,41]

$$\omega(p,h,E^*) = \frac{g(gE^* - A_{\rm ph})^{p+h-1}}{p!h!(p+h-1)!}f(h,E^*), \qquad (A16)$$

where the Pauli blocking factor $A_{\rm ph}$ is given by

$$A_{\rm ph} = \frac{p(p-1) + h(h-1)}{4},$$
 (A17)

and the finite-well-depth correction is given by

$$f(h, E^*) = \sum_{j=0}^{h} (-1)^j {\binom{h}{j}} \left(\frac{E^* - j * E_F}{E^*}\right)^{h-1} \\ \times \theta(E^* - j * E_F).$$
(A18)

We rewrite this density as

$$\omega(p, h, E^*)\Delta E = (g\Delta E)^{p+h}\mathcal{N}(p, h, N^*), \qquad (A19)$$

where

$$\mathcal{N}(p,h,N^*) = \frac{(N^* - A_{\rm ph}/(g\Delta E))^{p+h-1}}{p!h!(p+h-1)!} f(h,N^*), \quad (A20)$$

and

$$f(h, N^*) = \sum_{j=0}^{h} (-1)^j {\binom{h}{j}} \left(\frac{N^* - j * N_F}{N^*}\right)^{h-1} \\ \times \theta(N^* - j * N_F).$$
(A21)

In the unified model, the energy interval ΔE is taken to be the spacing between states. We then have $g\Delta E = r \approx 3$.

3. Emission

The partial width for emission of a particle of energy *e* and separation energy *B* is given in the exciton model by [11]

$$\frac{d\Gamma_e}{de} = \frac{g_s \mu}{\pi^2 \hbar^2} e\sigma_{abs}(e) \frac{\omega(p-1,h,E^*-B-e)}{\omega(p,h,E^*)}, \quad (A22)$$

where g_s is the spin multiplicity of the emitted particle, μ is the reduced mass of the particle and the residual nucleus, and σ_{abs} is the absorption cross section of the inverse process.

Taking $e = N_{sc}\Delta E$ and $E^* - B - e = N_f^*\Delta E$, we rewrite this as

$$\frac{d\Gamma_e}{d\varepsilon}\Delta E = \frac{g_s\mu}{\pi^2\hbar^2}\sigma_{abs}(N_{sc}\Delta E)N_{sc}(\Delta E)^2 \\ \times \frac{1}{g\Delta E}\frac{\mathcal{N}(p-1,h,N_f^*)}{\mathcal{N}(p,h,N^*)}.$$
 (A23)

In the unified model, the ratio of numbers of states is accounted for through the explicit counting of the states. The remaining product, that of the Weisskopf factor and the inverse factor of $r = g \Delta E$, is taken to be the partial emission width of the single-particle states.

4. Internal transition densities

The internal transition densities that enter the exciton model, known as the densities of available states, satisfy the relation [11,14,42]

$$\omega(p, h, E^*) \omega_+(p, h, E^*) = \omega(p+1, h+1, E^*) \times \omega_-(p+1, h+1, E^*) \approx \frac{(p+1)(h+1)(p+h)}{2} f(h, E^*) \times g \, \omega(p+1, h+1, E^*).$$

We then have approximately

$$\omega_{+}(p,h,E^{*}) \approx g \frac{(p+1)(h+1)(p+h)}{2} \times f(h,E^{*}) \frac{\omega(p+1,h+1,E^{*})}{\omega(p,h,E^{*})}$$
(A24)

or

$$\omega_{+}(p,h,E^{*})\Delta E \approx (g\Delta E)^{3} \frac{(p+1)(h+1)(p+h)}{2} \times f(h,N^{*}) \frac{\mathcal{N}(p+1,h+1,N^{*})}{\mathcal{N}(p,h,N^{*})}, \quad (A25)$$

and

$$\omega_{-}(p,h,E^*) \approx g \, \frac{ph(p+h-2)}{2} f(h-1,E^*)$$
 (A26)

or

$$\omega_{-}(p,h,E^*)\Delta E \approx (g\Delta E) \frac{ph(p+h-2)}{2} f(h-1,N^*).$$
(A27)

The density of available states that does not change the exciton number is given by

$$\omega_0(p,h,E^*) \approx g \, \frac{p(p-1) + h(h-1) + 4ph}{2(p+h)} (gE^* - A_{\rm ph})$$
(A28)

or

$$\omega_0(p, h, E^*) \Delta E \approx (g \Delta E)^2 \frac{p(p-1) + h(h-1) + 4ph}{2(p+h)} \times (N^* - A_{\rm ph}/(g \Delta E)) \,. \tag{A29}$$

With the exception of the factor $r^i = (g \Delta E)^i$, i = 1, 2, 3, the density of available states is accounted for in the unified model by explicit counting of each of the possible energy-conserving two-body transitions.

The partial widths for internal transitions are written in terms of the densities and the average squared matrix element $|M|^2$ as

$$\Lambda_{\pm,0}(p,h,E^*)\Delta E = 2\pi |M|^2 \omega_{\pm,0}(p,h,E^*)\Delta E.$$
 (A30)

In the unified model, the partial width for an individual transition is thus taken to be $2\pi |M|^2 r^i$, i = 1, 2, 3.

APPENDIX B: MONTE CARLO SOLUTION OF THE MASTER EQUATION

The master equation describing pre-equilibrium nucleon emission can be written as

$$\hbar \frac{dP_{na}}{dt} = \sum_{mb} \Lambda_{na,mb} P_{mb}(t) - \Gamma_{na} P_{na}(t), \qquad (B1)$$

where $P_{na}(t)$ is the instantaneous occupation probability of configuration na, $\Lambda_{na,mb}$ is the transition rate from configuration mb to configuration na, and Γ_{na} is the total rate (total width) of transitions from configuration i, given by

$$\Gamma_{na} = \sum_{e} \Gamma_{e,na} + \sum_{mb} \Lambda_{mb,na}, \qquad (B2)$$

where $\Gamma_{e,na}$ is the partial width for emission of a nucleon in an interval ΔE of the energy *e*.

We can write the instantaneous rate for particle emission at any given energy as a sum over the partial emission rate of each configuration times its occupation probability,

$$\frac{dS_e}{dt} = \frac{1}{\hbar} \sum_{na} \Gamma_{e,na} P_{na}(t).$$
(B3)

The spectrum of emitted particles is obtained by integrating this expression over time,

$$S_e = \frac{1}{\hbar} \int_0^\infty \sum_{na} \Gamma_{e,na} P_{na}(t) dt = \frac{1}{\hbar} \sum_{na} \Gamma_{e,na} \int_0^\infty P_{na}(t) dt.$$
(B4)

To evaluate this, it is convenient to suppress indices by using a vector-matrix notation. To do so, we treat the occupation probabilities as a vector \vec{P} , where each of the components corresponds to the occupation probability of a configuration. The transitions $\Lambda_{na,mb}$ and total widths Γ_{na} can be written as matrices Λ and Γ , with the latter diagonal. We can then rewrite the solution to the master equation as

$$\vec{P}(t) = \exp[-(\Gamma - \Lambda)t/\hbar]\vec{P}_0, \tag{B5}$$

where P_0 is the initial probability distribution.

To write an expression for the emission spectrum, we write the partial emission widths $\Gamma_{e,na}$ as a vector $\vec{\Gamma}_e$, with $\vec{\Gamma}_e^T$ being its transpose. We then have

$$S_e = \frac{1}{\hbar} \vec{\Gamma}_e^T \int_0^\infty \exp[-(\Gamma - \Lambda)t] \vec{P}_0 dt = \vec{\Gamma}_e^T \frac{1}{\Gamma - \Lambda} \vec{P}_0.$$
(B6)

We can rewrite the latter as

$$S_{e} = \vec{\Gamma}_{e}^{T} \Gamma^{-1} \frac{1}{1 - \Lambda \Gamma^{-1}} \vec{P}_{0}$$

= $\vec{\Gamma}_{e}^{T} \Gamma^{-1} (1 + \Lambda \Gamma^{-1} + \Lambda \Gamma^{-1} \Lambda \Gamma^{-1} + \cdots) \vec{P}_{0}.$ (B7)

Making the indices explicit, we have

$$S_{e} = \sum_{na} \frac{\Gamma_{e,na}}{\Gamma_{na}} \left(P_{0,na} + \sum_{mb} \frac{\Lambda_{na,mb}}{\Gamma_{mb}} P_{0,mb} + \sum_{mb,lc} \frac{\Lambda_{na,mb}}{\Gamma_{mb}} \frac{\Lambda_{mb,lc}}{\Gamma_{lc}} P_{0,lc} + \cdots \right).$$
(B8)

The Monte Carlo solution to the master equation mimics this form. Given the configuration na at any iteration, one considers the differential branching ratios for emission and for internal transitions,

$$\frac{\Gamma_{e,na}}{\Gamma_{na}}$$
 and $\frac{\Lambda_{mb,na}}{\Gamma_{na}}$, (B9)

observing that

$$\sum_{e} \frac{\Gamma_{e,na}}{\Gamma_{na}} + \sum_{mb} \frac{\Lambda_{mb,na}}{\Gamma_{na}} = 1.$$
(B10)

A transition to a new configuration *mb* or an emission is chosen randomly according to its branching ratio by (1) ordering the

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branching ratios, (2) choosing a random number between 0 and 1, and (3) choosing the new configuration or emission that corresponds to the random number from the ordered set of branching ratios. Thus the first iteration furnishes one of the

$$\frac{\Gamma_{e,na}}{\Gamma_{na}}$$
 or $\frac{\Lambda_{mb,na}}{\Gamma_{na}}$, (B11)

from an initial state na, while the second iteration furnishes one of the

$$\frac{\Gamma_{e,mb}}{\Gamma_{mb}} \frac{\Lambda_{mb,na}}{\Gamma_{na}} \quad \text{or} \quad \frac{\Lambda_{lc,mb}}{\Gamma_{mb}} \frac{\Lambda_{mb,na}}{\Gamma_{na}}, \quad (B12)$$

and so forth. Summing and normalizing a large number of cases then produces the solution to the master equation.

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