# Precompound Monte-Carlo model for cluster induced reactions

M. Blann[1] and M. B. Chadwick[2]
[1]*7210E Calabria Court, San Diego, California 92122*
[2]*University of California, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*
(Received 2 August 1999; revised manuscript received 6 January 2000; published 2 August 2000)

We present an algorithm for Monte-Carlo selection of exciton energies for reactions induced by clusters. Reaction mechanisms are addressed that involve a dissolution of the cluster into its constituent nucleons followed by the initiation of a preequilibrium cascade. Calculated single differential spectra and excitation functions for $^{93}$Nb$(\alpha,xn)$ reactions are compared with experimental results to illustrate use of this method. Some advantages of exclusive computational techniques over analytic inclusive methods are summarized.

PACS number(s): 24.10.Lx, 25.40.Hs, 25.55.Hp

## I. INTRODUCTION

Precompound models based on an assumed equilibration sequence of intranuclear two body interactions have proven valuable as a tool in the interpretation of a variety of nuclear reactions [1,2]. These models have in common a summation of contributions from ever more complicated (in terms of particle-hole excitations) configurations contributing to the decay process of the excited nuclei, prior to achieving a quasiequilibrium.

It has been demonstrated that for nucleon induced reactions, the three quasiparticle excitation is produced with nearly equal *a priori* energy sharing between the three ''excitons,'' if calculated using *N-N* scattering cross sections in a Fermi gas [3]. Thus for the first term in the usual precompound decay models, the use of ''partial state densities'' based on exciton number [4] is justified. However, Bisplinghoff [5] clearly illustrated that precompound models in use were inconsistent in their use of higher order (than the first three-exciton result) exciton density prescriptions, if the two body transition assumption was made. A second shortcoming of existing precompound models was a difficulty in treating multiple emission of precompound nucleons from a single nucleus, and in treating exclusive reactions for differential cross sections.

Both the aforementioned shortcomings of preequilibrium models have been removed, for nucleon induced reactions, by application of Monte-Carlo algorithms, in what we have called the hybrid Monte-Carlo simulation (HMS), or more accurately the precompound Monte-Carlo simulation model [6,7]. The latter name is preferable as the treatment is not a Monte-Carlo version of the hybrid model [8]. Rather it uses the fact that the three-exciton configuration produced by the interaction of a nucleon with a nucleus in a two-body process should give approximately the nucleon energy distribution represented by the three-exciton density function [4], and by difference, of the two exciton density. In the Monte-Carlo approach [6], each successive scattering of a nucleon is treated as producing a new three-exciton configuration, consistent with the two-body assumption. This avoids use of the higher order exciton densities which Bisplinghoff demonstrated were inconsistent with population by a two body mechanism. This Monte-Carlo approach may be used to calculate unlimited multiplicities of precompound emitted nucleons and may have various ''gates'' put on emitted nucleons. In other words, our Monte-Carlo approach allows unlimited emission of preequilibrium ejectiles (so-called multiple preequilibrium), and it can be used to compute exclusive reactions where specific correlations between the ejectiles are of interest.

A limitation of this approach was that it was formulated only for nucleon induced reactions, not for heavier cluster induced reactions. In this paper we present a simple algorithm for cluster/light-ion induced reactions, intended to extend the benefits of the Monte-Carlo approach to these cases. Our main goal in this work is to document the method, so that it will be available to those wishing to use it. We will use alpha induced reactions with which to compare our results, because many are available in the literature; there are particle spectra for different incident energies, and many excitation functions from which to choose. However, as elegantly demonstrated by Gadioli *et al.* [9], and in earlier work by Lanzafame *et al.* [10,11] there are other competing direct reactions with any complex projectile induced reaction, which must be considered. This point will be discussed when comparisons are made with experimental results; for a comprehensive discussion we refer to the work of Gadioli *et al.* [9].

We will first present the assumptions used in extensions to cluster induced reactions, and refer to earlier results which support (but can never prove) the formulation adopted. We then present the algorithm used to extend this model to Monte-Carlo implementation described in [6], and finally present a few comparisons with experimental data to give some validation to these results. Our purpose is mainly to present the method, rather than to exhaustively compare it with a large body of data. This is because we expect it to give results similar to the Boltzmann master equation and hybrid model for inclusive spectra (since the same n-exciton partition function is used in these cases) and many results have been published for these cases, with good agreement with experiment for incident ions as heavy as $^{40}$Ca [12–16].

## II. MONTE-CARLO ALGORITHMS FOR CLUSTER INDUCED REACTIONS

To treat precompound reactions induced by light ion clusters, one must make an assumption about the initial energy

 

partition upon the two nuclei (nuclear potentials) interacting. An early treatment of the problem made the assumption that once the two nuclei (target and projectile) were in the same potential field, the projectile nucleons might, feeling the whole field, act as though they were free to move in that field [12,13]. It was assumed that in doing so, their incident ''beam'' energy per nucleon, coupled with their random Fermi motion, would give a distribution of nucleon energies having equal *a priori* probability [12]. They could either be emitted, or they could rescatter in two body interactions. In this scenario, the initial distribution function would be represented by an exciton distribution function [4] with a number of excitons equal to the mass number of the projectile. While this was presented as an intuitive guess, its trial gave good agreement with a large body of experimental data, for incident ions as high as $^{40}$Ca, in use in the hybrid and Boltzmann master equation models. Indeed, predictions made about light and heavy ion precompound decay, years before measurements were possible (due to accelerator development) [17] were later shown to give very good guidance as to phenomena observed in later years. Scobel [18] demonstrated in a Monte-Carlo calculation, that the random coupling of beam and Fermi motion in a projectile does indeed produce a distribution very near the ''$n$'' exciton function we assumed. Our purpose in this paper is to demonstrate how this may be used in a Monte-Carlo implementation so as to yield a consistent model permitting unlimited precompound multiplicity (which is important for heavy ion reactions) and calculation of exclusive yields while retaining use of three-exciton formulas for treating the $N$-$N$ rescattering part of the cascade process.

With the equal *a priori* assumption above, the $n$ exciton formula may be used to give the number $N$ of equally likely combinations of $n$ excitons at excitation $E$, with $g$ equidistant levels per MeV as

$$N(E)=\frac{(gE)^{n-1}}{p!h!(n-1)!}, \tag{1}$$

where $p,h$ are the particle and hole numbers. If we select an exciton with energy $e$ above the Fermi level, and ask for the probability $P(e)$ of finding an exciton with that energy, we find (where $U=E-e$)

$$P(e)=\frac{1}{N(E)}\frac{(gU)^{n-2}}{(p-1)!h!(n-2)!}\frac{g}{p}. \tag{2}$$

We may then inquire as to the expectation of a second particle from the original $n$-exciton configuration by repeating the process for a configuration of $(n-1)$ excitons at excitation $U$, etc., until there are but two excitons remaining. These may have their energies selected between the remaining excitation at random. For Monte-Carlo sampling we must express the probability information given by successive applications of Eq. (2) in terms of the energy of an exciton picked from the equally probable distribution [Eq. (1)] by picking a random number $x$ between 0 and 1 [we note that the integral of Eq. (2) for $e$ between 0 and $E$ is 1]. Each energy has a probability associated with it, as given by Eq. (2), so each interval covered by $x$ must have a relative length as a fraction of 1 proportional to that probability. This is fulfilled if we define

$$x=\int_0^e P(e')de' \tag{3}$$

and then we may solve for the energy $e$ selected by the random number $x$ as

$$e=E(1-(1-x)^{1/(n-1)}). \tag{4}$$

Making the algorithm general to include both particle and hole excitons, we first define the total neutron, proton particle exciton numbers, and the hole number. The sum of these is $n$. We define the hole probability as the hole number, $h$, divided by $n$. A random number is used to select the first exciton as a particle or a hole, depending on whether $x$ is greater or less than the hole probability. If a particle exciton is selected, a random number is similarly used to select whether the exciton is a neutron or a proton, based on the fraction of the exciton particle population occupied by each. In the case that a hole exciton is selected, a random number is used to select a neutron or proton hole. A random number is selected to pick the particle or hole energy using Eq. (4); if a hole, the energy is tested to see if it exceeds the potential well depth; if it does, another random number/energy is selected until this constraint is satisfied.

Once an exciton type and energy have been selected as described above, the neutron/proton/exciton numbers are appropriately decremented, the excitation is decremented by that of the selected exciton, and the selection process is continued for the next exciton. When only two excitons remain, the energy of the first is selected by a random number, and that of the final exciton is selected by difference to conserve energy.

The energies of all excitons resulting from the primary interaction of the incident cluster with the target nucleus are calculated in this manner. Each is now analogous to a nucleon projectile which may initiate a reaction (as described in Refs. [6,7]), but each must first be multiplied by the branching ratio for emission or rescattering. In the case of a Monte-Carlo calculation, the ratio

$$Rc(e)=\frac{lc(e)}{lc(e)+lp(e)} \tag{5}$$

represents the probability that an exciton at energy $e$ above the Fermi energy is emitted rather than rescattering, $lc(e)$ being the emission rate, and $lp(e)$ the damping rate. Then if a random number is greater than $Rc(e)$, the exciton is assumed to initiate a cascade with excitation energy $e$, i.e., a two particle–one hole configuration is formed, treated by the Monte-Carlo formalism for nucleon induced reactions which has previously been described [6]. In the case that the random number is less than $Rc(e)$, the exciton is presumed to be emitted into the continuum and is added to the emission spectrum. This procedure is followed for each of the excitons resulting from the initial cluster-nucleus interaction.

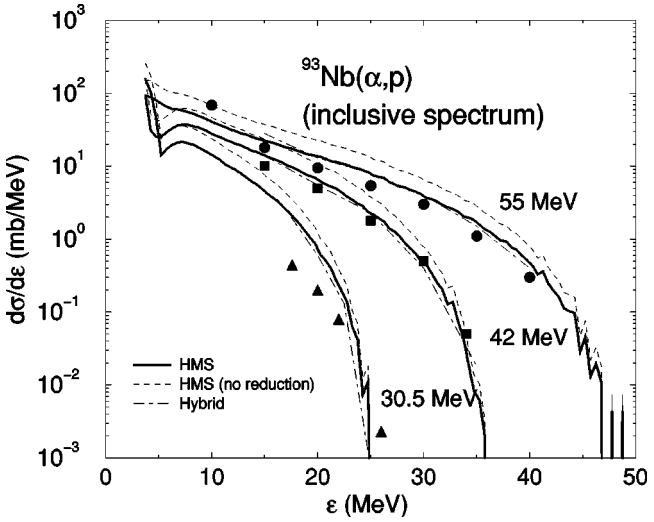


FIG. 1. Experimental and calculated $(\alpha,p)$ spectra on $^{93}$Nb. Triangles are points for 30.5 MeV incident alpha particles from [19]; squares are for 42 MeV alpha particles from [20], and circles are for 55 MeV alpha particles from [21]. Solid lines are the results of the HMS Monte-Carlo simulation described in this work, having been reduced by a factor of 0.6 to account for reaction flux estimated to be lost to other low-momentum transfer reactions (see text, and discussions by Gadioli *et al.* [9]). The HMS results without any such reduction are shown as dashed lines. Additionally, the dashed-dot lines show results using the hybrid model presented in Ref. [2].

Comparing precompound spectra with calculated results has often shown that better agreement results if a pairing correction is made to parent/daughter excitations in the distribution functions. We mention this as an empirical observation rather than a theoretical principle. The algorithm with pairing correction terms becomes

$$e=[E-\Delta(\text{daughter})]-[E-\Delta(\text{parent})](1-x)^{1/(n-1)}, \tag{6}$$

where $\Delta$ (daughter/parent) represents the daughter/parent pairing energy. We have used Eq. (6) in calculations to be presented in this work; however differences due to pairing corrections are rather trivial for the examples to be presented.

### III. RESULTS AND DISCUSSION

It is important to note that the formalism described here is appropriate for describing only a fraction (albeit a significant fraction) of all reaction mechanisms that can take place. Specifically, it addresses reaction mechanisms that lead to a preequilibrium cascade of nucleon-nucleon interactions following the dissolution of the alpha particle. As discussed by Gadioli and others [9–11], additional reaction mechanisms are present due to the higher partial waves of the entrance channel, such as inelastic scattering of the alpha particle with the nucleus as a whole, pickup reactions, and binary fragmentation. From the detailed analysis by Gadioli *et al.* [9] of the various contributing reaction mechanisms in $\alpha+^{93}$Nb reactions, we estimate that approximately 60% of the reaction cross section leads to alpha particle dissolution followed by a

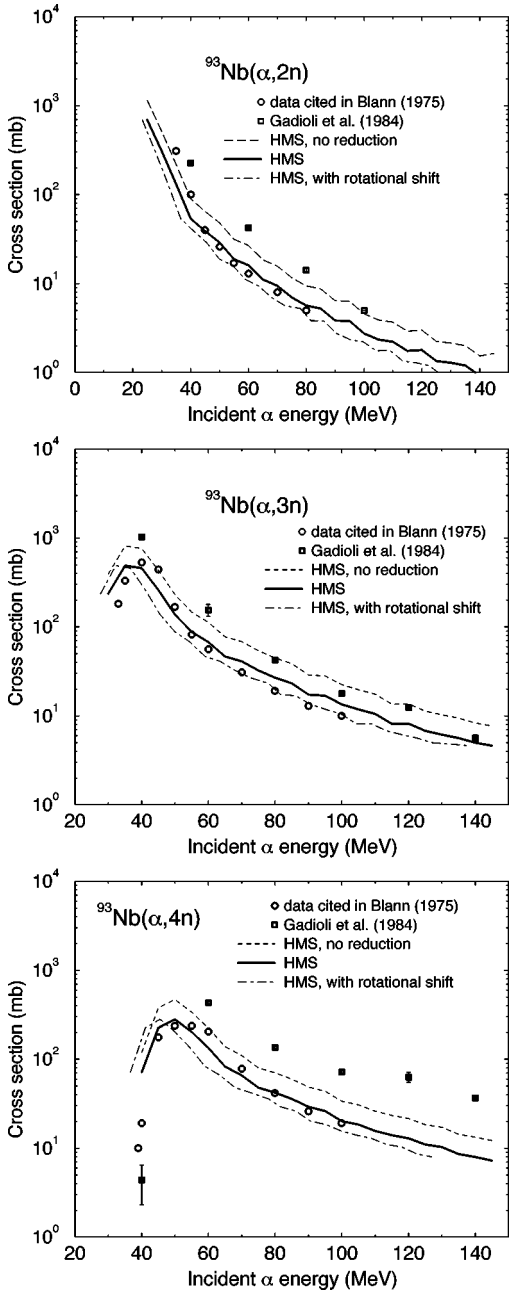


FIG. 2. Experimental and calculated excitation functions for alpha induced reactions of $^{93}$Nb. Open circles and squares are experimental results from [22,23] and [9] respectively for the $(\alpha,xn)$ excitation functions for $x=2$, 3, 4. Solid curves are the results of the HMS Monte-Carlo simulation described herein, having been reduced by a factor 0.6 to account for reaction flux lost to other mechanisms. The unreduced HMS results are shown as dashed lines. Dashed-dot lines represent calculated results shifted downward by the average rotational energy at each incident energy.

preequilibrium cascade. In the results shown below we apply this reduction factor (0.6) to the total reaction cross section. We have ignored the weak energy-dependence expected for this reduction factor because it is significantly smaller than the uncertainty in its magnitude, which is estimated to be about 15%.

We present comparisons of particle spectra (single differential cross sections) and of excitation functions for alpha

induced reactions on $^{93}$Nb. In Fig. 1 experimental results are shown for incident alpha energies of 30.5 [19], 42 [20], and 55 MeV [21]. In Fig. 2 excitation functions measured by two different groups for incident energies up to 140 MeV [22,23,9] are shown. It has been found empirically [2] that for odd *A* targets, alpha induced reactions are best represented by initial 5 exciton configurations. Results presented therefore were calculated assuming a three proton, two neutron set of initial excitons, i.e., it is assumed that the unpaired proton in the target was excited in the initial interaction. This is pure conjecture motivated by the empirical observations of past analyses of alpha induced reactions.

In Fig. 1 we see good agreement between calculated (solid line) and experimental results for the shapes and magnitudes of the spectra at 42 and 55 MeV incident alpha energy. The agreement with the 30.5 MeV incident alpha data is poor both respect to shape and magnitude; however in terms of the experimental uncertainties of the four measured points, the calculated results are not unreasonable. In this figure we also show HMS results in which the reaction cross section has not been reduced, to serve as a reminder to the reader that the HMS results include an estimate of flux lost to other processes. Finally, we also reproduce the hybrid model calculations presented in Ref. [2] for comparison. While the quality of the HMS and the hybrid model results appear to be similar, with respect to agreement with the data, we remind the reader that the HMS results are far richer in the sense that they preserve all correlation information between ejectiles. (This cannot be seen in Fig. 1 since the measurements are of the inclusive emission spectrum.)

Comparisons more sensitive to details of the multiple precompound decay mechanism may be found in excitation functions, e.g., Fig. 2. We have plotted the results calculated as described herein as solid curves in Fig. 2, labeled ''HMS.'' Again, we also plot for comparison results in which the reaction cross section was not reduced. Our evaporation calculation does not contain the rotational energy correction (yrast cascade enhanced by angular momentum) which we would get from a Hauser-Feshbach calculation, or from an *s*-wave evaporation approximation. We have therefore shown our results shifted downward by the average rotational energy for each incident alpha energy as a dashed line. This will overestimate the yrast cascade effect, but give guidance as to an upper limit of its effect. The calculated excitation functions (solid lines) lie in between the two experimental sets shown, generally exhibiting better agreement with the data of Bisplinghoff *et al.* [22].

## IV. CONCLUSIONS

We have presented a straightforward, and computationally fast algorithm which will allow precompound Monte-Carlo calculation of reactions induced by clusters for which it is assumed that the cluster ''dissolves'' in the field of the target nucleus and gives an energy conserving equal *a priori* *n*-exciton distribution resulting from coupling of beam and Fermi momenta. This was shown to be a good description in earlier works within both the hybrid model and the Boltzmann master equation. The Monte-Carlo formulation of the preequilibrium process leads to three main formal improvements in the theory: use of correct three-exciton distributions for all stages of the scattering process; allowance of unlimited precompound emissions; and preservation of correlations between ejectiles emitted in a given event.

This algorithm has been incorporated into the nuclear modeling code HMS-ALICE, and has been shown to give reasonably good results in comparisons with several experimental data sets for alpha induced reactions. Many more comparisons are desirable, in particular to test reactions for which multiple precompound decay channels are important, and for coincidence experiments exploiting the capabilities of event mode models to predict gated (exclusive) results where correlations are important. Comparisons with heavy ion induced reactions will be worthwhile; based on the success of the Boltzmann master equation for heavy ion reactions using the same algorithm for the initial nucleon distribution [12–16], we expect the algorithm presented herein might be useful for treating heavy ion reactions where fusion occurs.

## ACKNOWLEDGMENT

The authors wish to thank Dr. P. Oblozinsky for useful comments.

[1] E. Gadioli and P. E. Hodgson, *Pre-Equilibrium Nuclear Reactions* (Oxford University Press, Oxford, UK, 1992).
[2] M. Blann, Annu. Rev. Nucl. Sci. **25**, 123 (1975).
[3] M. Blann and H. Vonach, Phys. Rev. C **28**, 1475 (1983).
[4] T. Ericson, Adv. Phys. **9**, 423 (1960).
[5] J. Bisplinghoff, Phys. Rev. C **33**, 1569 (1986).
[6] M. Blann, Phys. Rev. C **54**, 1341 (1996).
[7] M. Blann and M. B. Chadwick, Phys. Rev. C **57**, 233 (1998).
[8] M. Blann, Phys. Rev. Lett. **27**, 337 (1971).
[9] E. Gadioli, E. Gadioli Erba, J. J. Hogan, and B. V. Jacak, Phys. Rev. C **29**, 76 (1984).
[10] F. M. Lanzafame and M. Blann, Nucl. Phys. **A142**, 559 (1970).
[11] M. Blann and F. M. Lanzafame, Nucl. Phys. **A142**, 545 (1970).
[12] M. Blann, Nucl. Phys. **A235**, 211 (1974).
[13] M. Blann, R. R. Doering, A. Galonsky, D. M. Patterson, and F. E. Serr, Nucl. Phys. **A257**, 15 (1976).
[14] M. Blann, Phys. Rev. C **23**, 205 (1981).
[15] M. Blann, Phys. Rev. C **35**, 1581 (1987).
[16] M. Blann and B. A. Remington, in *Proceedings of the International Conference on Nuclear Reaction Mechanisms*, Varenna, Italy, 1988, edited by E. Gadioli (Universita Degli Studi di Milano, Milan, 1988), p. 184.
[17] M. Blann, Phys. Rev. C **31**, 1245 (1985).
[18] W. Scobel, in *6th Adriatic Conference on Nuclear Physics*,

Dubrovnik, 1987, edited by N. Cindro, W. Greiner, and R. Caplar (World Scientific, Singapore, 1987), p. 267.
[19] M. Blann, Annu. Rev. Nucl. Sci. **25**, 123 (1975), see Ref. [30] therein.
[20] R. W. West, Phys. Rev. **141**, 1033 (1966).
[21] A. Chevarier, N. Chevarier, A. Demeyer, G. Hollinger, R. Pertosa, and Tran Minh Duc, Phys. Rev. C **8**, 2155 (1973).
[22] J. Bisplinghoff, Annu. Rev. Nucl. Sci. **25**, 123 (1975), see Ref. [79] therein.
[23] H. Stockhorst, W. Feiedland, and J. Ernst, in *Proceedings of the International Conference on Nuclear Reaction Mechanisms*, Varenna, Italy, 1982, edited by E. Gadioli (Universita Degli Studi di Milano, Milan, 1982).