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A Microscopic semi-classical model of nucleon-induced pre-equilibrium reactions.

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Abstract. We present a microscopic description of the nucleon-nucleon collision cascade that permits the modeling of typical cascade and exciton descriptions of the process. Each configuration of particles and holes is treated explicitly and transitions induced by energy-conserving two-body collisions are considered. We can reproduce the extreme limits assumed in cascade and exciton type models. Although the microscopic description of the interaction chain can be written in the form of a master equation, the number of configurations is usually quite large and a Monte Carlo simulation method is used to obtain solutions.

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Introduction

Pre-equilibrium emission plays an important role in nucleon-induced reactions at incident energies above about 10 MeV. Although quantum mechanical models of these reactions have been developed [1,2], most calculations for technological applications still rely on older, but very successful, semi-classical models of the cascade [3,4] or exciton [5,6] type. Yet, these models assume radically different properties of the chain of nucleon-nucleon interactions that leads to pre-equilibrium emission [7].

Semi-classical pre-equilibrium reaction models are normally formulated on the basis of a set of 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, a number of the particles occupy states above the Fermi energy, leaving the same number of holes

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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. We define an exciton class as a set of configurations with the same number of particles and holes.

As discussed in Ref. [7], models of the cascade type, the hybrid model [4], as well as its more modern version, the hybrid Monte Carlo simulation (HMS) [5], neglect all transitions between configurations of the same exciton class. The HMS model describes the reaction cascade in terms of a sequence of one particle-one hole (1p-1h) excitations. These excitations are taken to be well-defined configurations that are altered only when the particle or hole participate in a subsequent collison or the particle is emitted.

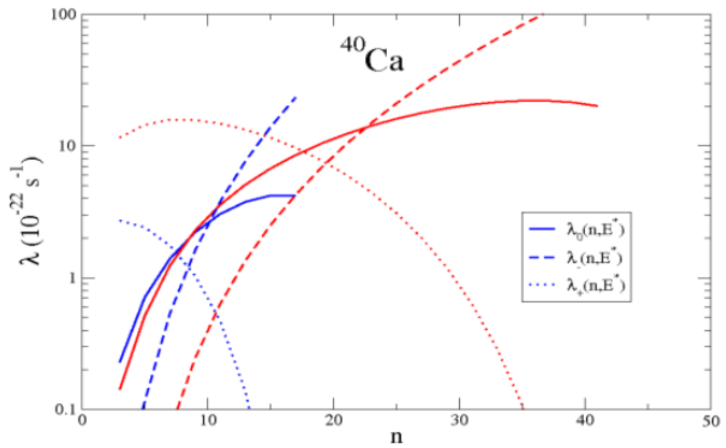

Fig. 1. Exciton model transition rates (arbitrary units) at excitation energies of 20 MeV (blue) and 100 MeV (red).

Models of the exciton type assume that the configurations of an exciton class are in equilibrium at all stages of the reaction cascade. Exciton models thus define transition rates using state [8] and transition [9] densities for the exciton classes. However, for equilibrium to be established, the transition rate between configurations of a given exciton class must necessarily be much larger than the transition rates between classes. We can test this hypothesis within the exciton model itself, since it permits the calculation of the transition rate between configurations of the same class, $\lambda_0(n)$, n being the exciton number, as well as the rates of transitions that increase and decrease the exciton number, $\lambda_+(n)$, and $\lambda_-(n)$, respectively.

In Fig. 1, we display the transition rates (in arbitrary units) for the system nucleon + ^{40}Ca as a function of the number of excitons n, at excitation energies of 20 and 100 MeV. At all energies, we see that the transition rate $\lambda_0(n)$ is smaller than or about equal to the transition rate $\lambda_+(n)$ at low exciton number. Thus we do not expect the equilibrium hypothesis of the exciton model to be satisfied at the initial stage of the reaction cascade.

In the following, we develop a unified microscopic model that permits us to simulate both the cascade and exciton type models, as well as intermediate ones, and compare the results of numerical simulations.

The model

We use a uniformly-spaced single-particle spectrum in the model, 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 thus a 1p-1h one, with the hole at the Fermi energy and the particle (the projectile) occupying the single-particle state closest in the total excitation energy $E^* = E_n + B$ 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. We label each particle-hole configuration by a letter from the beginning of the alphabet a, b, c,... as well as a class label l, m, n, ... denoting the exciton number, that is, the total number of particles and holes. The class label is actually redundant, being completely determined by the configuration, but is useful when considering the exciton-model limit. We thus denote the occupation probability of a typical configuration as P_{na}.

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

$$\hbar \frac{dP_{na}}{dt} = \sum_{mb} \Gamma_{na,mb} P_{mb} - \Gamma_{na} P_{na}. \tag{1}$$

The total decay width of the configuration na is given in terms of the partial transition widths $\Gamma_{lc,na}$ and partial emission widths $\Gamma_{e,na}$ by

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

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

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

The number of configurations is usually quite large. In the simple case of a nucleon incident on ^{16}O at 20 MeV, about 600 configurations and, thus, 600 coupled equations are required, while at 100 MeV, about 43000 configurations are involved. In the case of a nucleon incident on ^{56}Fe at 100 MeV, the number of configurations is on the order of 130 million. Direct solution of the equations is simply not viable in general. We use instead a Monte Carlo simulation method, which has the additional advantage of being easily parallelizable.

Emission. We estimate emission using the usual Weisskopf-Ewing expression. We take the partial width for nucleon emission in an interval ΔE of the emission energy e from the configuration na to be

$$\Gamma_{e,na} = \frac{d\Gamma_{e,na}}{de}\Delta E = \frac{2g_s\mu}{\pi\hbar^2} e\sigma_{abs}(e)\Delta E, \tag{4}$$

if the configuration contains a particle at an excitation energy of $e + B$, 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 then the sum over the partial widths of each of the particles that can be emitted.

Transitions. We consider transitions induced by energy-conserving two-body collisions and denote the partial width for such a transition from mb to na as $\Gamma_{na,mb}$. We assume microscopic reversibility, so that $\Gamma_{na,mb} = \Gamma_{mb,na}$. Since the transitions are due to two-body interactions, the nonzero partial transition widths will be those that increase the exciton number by 2, $\Gamma_{n+2a,nb}$, those that leave it the same, $\Gamma_{na,nb}$, and those that decrease it by 2, $\Gamma_{n-2a,nb}$. The two-body collision inducing the transition from a configuration mb to a configuration na 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, we can then associate a single value to all non-zero partial widths. In the following, we call this model the natural one.

HMS and exciton model limits. By varying the value used for different classes of states, we can study the effects of the different hypotheses of models in use today. By taking $\Gamma_{na,nb} \to 0$, we eliminate transitions between configurations in the same exciton class. We will denote this limit as the HMS model.

When the partial widths for transitions within an exciton class are much bigger than those between classes,

$$\Lambda_{na,nb} >> \Lambda_{na,mb},\, \Lambda_{mb,na} \qquad\qquad m \neq n, \tag{5}$$

we would expect the configurations within each exciton class to reach equilibrium before transitions take place between exciton classes. In this limit, the model should reduce to the usual exciton model, in which system evolution and emission rates depend only the populations of the exciton classes and not those of the individual configurations. In the following, we will denote as Monte Carlo (MC) exciton calculations those 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.

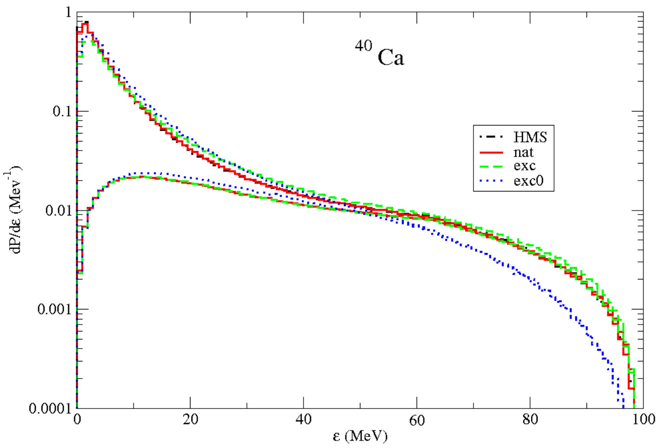

Fig. 2. Spectrum of first and total nucleon emission from nucleon + ^{40}Ca at an incident energy of 100 MeV.

Numerical Results

In this section, we compare the results of calculations using the different model hypotheses discussed above. In Fig.2, we show the spectrum of the first and total nucleon emisson from the system nucleon + ^{40}Ca at an incident center-of-mass-energy of 100 MeV. The curve labeled exc (green) refers to the usual exciton model with a hole frozen at the Fermi surface. This hole is free in the exciton model calculation labeled exc0 (blue). The first emssion spectrum is essentialy equal to the total spectrum above about 50 MeV. At lower energies, the total emission spectrum greatly exceeds that of the first emission. We see that three of the four simulations give fairly similar results. The HMS (black curve) and natural (red curve) simulations are in such close agreement that they are superimposed on one another. The two are also in fair agreement with the exciton calculations (green curve). However, the agreement of the exciton calculations with the HMS and natural ones is only obtained by freezing the initial hole at the Fermi energy until after the first emission had occurred. The exciton model thus depends on a conceptual inconsistency: one must freeze one degree of freedom, the hole at the Fermi energy, but require that the others interact strongly within the exciton class.

Conclusions

We have developed an unified microscopic model of semi-classical nucleon-induced pre-equilibrium reactions that permits us to simulate the radically different hypotheses of cascade and exciton type models, as well as intermediate ones. We simulate an exciton type model by making the partial widths for transitions between configurations of the same exciton class much greater than those that change the class, and verified that the Monte Carlo simulation of the exciton model produces the same results as the exciton model obtained by assuming equilibrium among configurations and reducing the problem to one of transitions between classes.

We find the results of the natural model to be much closer to those of the cascade type model than to the exciton one. In addition, we find that the exciton model is capable of producing results similar to the other two only when two inconsistent hypotheses are used simultaneously: One must freeze a hole at the Fermi energy yet assume that the other degrees of freedom interact strongly within the class. Although the exciton model will certainly continue to be used due to its simplicity, work on models that are more consistent conceptually is warranted.

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