A Monte Carlo model of deuteron emission in pre-equilibrium nuclear reactions

E A Teixeira and B V Carlson
Dep. de Física, Instituto Tecnológico de Aeronáutica, São José dos Campos, SP, Brazil
E-mail: estevao@ita.br

Abstract. Nucleon-induced pre-equilibrium reactions are important in many applications of nuclear physics. About 20% of the particles emitted in such reactions are composites, such as deuterons and alpha particles. Deuterons are produced through emission from the compound nucleus, as well as through two important direct reaction mechanisms - “pick-up” and coalescence. Iwamoto and Harada developed a semi-classical pre-equilibrium model that describes both direct mechanisms as a generalization of coalescence. We have implemented the Iwamoto and Harada unified model of deuteron emission in Blann and Chadwick’s hybrid Monte Carlo model. This implementation was made in order to analyse data of reactions of the type (p,d), that is, proton induced reactions having deuterons as emitted particles, but our previous results were not satisfactory. In order to find a new approach for the deuteron emission, we are investigating an eikonal approximation to the phase space of Iwamoto and Harada model. We are also comparing our angular distributions with the experimental ones using DWUCK4. Nevertheless, our results are not satisfactory yet and our work is under development.

1. Introduction

Nucleon-induced pre-equilibrium reactions are important in the description and modeling of fast reactors, accelerator-driven systems (ADS) and radiotherapy with particle beams. The exciton model of pre-equilibrium reactions assumes the excitation of a chain of particle-hole states of the pre-compound nucleus that results from the fusion of the incident particle with the target (two particles and one hole, three particles and two holes, etc.) [1]. To estimate emission from the stage of n+1 particles and n holes, it assumes that each state of this kind is equally probable. However, Bisplinghoff demonstrated that in general this hypothesis is satisfied only for the initial configuration of two particles and one hole states [2].

With the goal of defining a pre-equilibrium reactions model without this defect, Blann developed a model called the “hybrid Monte Carlo” model (HMS), which takes into account the chain of particles and holes states of the exciton model through independent excitations of two particles and one hole [3, 4]. A detailed comparison between both models shows that while the exciton model assumes that the interaction between the configuration of n+1 particle and n hole states is so strong that these reach equilibrium before making another transition, the “hybrid Monte Carlo” model neglects any interaction between the particle - hole states of each configuration. Obviously, the physical case should lie between these two extremes.

About 20% of the pre-equilibrium emissions in these reactions correspond to composite particles, such as deuterons and alpha particles. An important reaction mechanism for the
production of deuterons is “pick-up”, in which an incident nucleon takes another nucleon from the target nucleus. Another pre-equilibrium deuteron production mechanism is coalescence [5, 6, 7], in which a deuteron is formed from two fast nucleons that are emitted close to one another in phase-space. In the context of the exciton model of pre-equilibrium reactions, Iwamoto and Harada developed a model that unifies these two mechanism of deuteron emission [8, 9, 10].

2. Iwamoto and Harada unified model

We started with the model proposed in Ref. [9], in which deuteron formation is represented by a quasi-classical phase space factor. As we were trying to reproduce their results, we found some inconsistencies in their calculations. With that, we tried to improve this model by making the necessary adjustments to implement it in Blann and Chadwick’s model, [4]. This implementation would allow us to obtain more realistic results in pre-equilibrium nuclear reactions.

Even with the treatment of the inconsistencies in the Iwamoto and Harada model, our results were not satisfactory. Our values did not fit with the experimental values and the results of the deuteron formation mechanisms did not follow the same pattern as the experimental data. As an example, our ratio of the deuteron pick-up partial emission widths and proton partial emission widths decreased with the increase of the target mass while the experimental data kept the same ratio.

3. Eikonal phase space

We decided to investigate an alternative approximation to the phase space as a way to improve our last results. With that, we have begun to investigate an eikonal phase space.

To begin, we calculate the one-step distorted-wave Born approximation (DWBA) amplitude of a proton-induced (p,d) reaction in the following way:

\[
\langle \vec{K}_d; h|T^{(1)}|\vec{K}_p \rangle = \int d^3r_d \int d^3r_p \phi_d \psi_d^{(-)} V(\vec{r}_d - \vec{r}_p) \phi_n \psi_p^{(+)},
\]

where \(\psi_d^{(-)}\) is the outgoing deuteron wave function and \(\psi_p^{(+)}\) is the incoming proton wave function. Both of these include the information of the plane wave plus the spherical wave that reach the detector. \(\phi_n\) is the neutron wave function and \(\phi_d\) is the internal wave function of the deuteron.

4. Preliminary results

We started analyzing the differential cross section for the (p,d) reaction on \(^{40}Ca\) in the 1\(d_3/2\) ground-state. However, our simulations did not achieve the same pattern as the experimental data [13].

In order to see why the differential angular cross section did not fit with the experimental data, we searched for the cause of the difference between the results. At first, we tested the \(t\rho\) potential against the optical potential that Ref. [13] uses.

In our work, the incident proton is subject to a potential represented by the \(t\rho\) approximation,

\[
U(\vec{r}) = -\frac{\hbar v}{2} \left[ \sigma_{pp} (i + \alpha_{pp}) \frac{Z}{A} + \sigma_{pn} (i + \alpha_{pn}) \frac{N}{A} \right] \rho_m(\vec{r}).
\]

with \(\sigma_{n_1n_2}^{T}\) being the total cross section and \(\alpha_{n_1n_2}\) a scattering phase factor, both energy dependent. \(\rho_m(\vec{r})\) is the target density distribution, \(v = \hbar k/\mu\), \(Z\) and \(N\) are the proton and neutron number of the nucleus of mass number \(A = Z + N\). We interpolated the values found in Ref. [14] to obtain \(\alpha\) and \(\sigma\).
In Ref [13], a phenomenological optical potential is used. It is given by

\[ V(r) = V_C(r_C) - V(e^x + 1)^{-1} - i \left( W - 4W_D \frac{d}{dr} \right) (e^{x'} + 1)^{-1} - \frac{\hbar c}{m_p c^2} \left( V_{SO} - \frac{1}{r} \frac{d}{dr} (e^{x''} + 1)^{-1} \sigma I \right), \tag{3} \]

where \( x = (r - R_0)/a_0 \), \( x' = (r - R')/a' \), \( x'' = (r - R'')/a'' \), with \( R_0 = r_0 A^{1/3} \), etc., and the Coulomb potential \( V_C \) is that for a uniformly charged sphere of radius \( R_C = r_C A^{1/3} \). \( W_0 \) and \( W_D \) are the volume and surface parts, respectively, of the imaginary potential, and \( V_{SO} \) is the real part of the spin-orbit potential, \( \sigma \) is the projectile spin and \( I \) is the orbital angular momentum. The values of the parameters are given in Ref. [13].

In Ref [13], the distorted-wave Born approximation (DWBA) code DWUCK (Distorted Wave University of Colorado Kunz) [15] was used to analyze the differential cross section. As we are trying to build our code and using their experimental values as our source, we decided to compare results.

As our next step, we expect to conclude our comparison of the optical model potential and the \( t\rho \) potential. With that, we expect to have a good idea of how the \( t\rho \) approximation should behave in our differential cross section results. This step is important in order to validate the phase space that we are studying. Our hope is to improve the calculations of our model of deuteron emission in pre-equilibrium reaction.

### Figure 1.
Comparison between the \( t\rho \) approximation and the optical potential used in Ref. [13]. The abscissa represents the nucleus radius in fm and the ordinate represents the potential value in MeV. The red vertical line represents the target radius.

In Fig. 1, one can see that our potential is in a good agreement with the optical potential just at large radii but much deeper at smaller radii.

In Ref. [13], the distorted-wave Born approximation (DWBA) code DWUCK (Distorted Wave University of Colorado Kunz) [15] was used to analyze the differential cross section. As we are trying to build our code and using their experimental values as our source, we decided to compare results. In Fig. 2, one can see their experimental values (dots) and our calculations using their values input in DWUCK4 (line). In their work, they used an adiabatic potential for the deuteron channel but we did not include it in our input. It may be what causes the difference between our results, but such a conclusion is preliminary.

As our next step, we expect to conclude our comparison of the optical model potential and the \( t\rho \) potential. With that, we expect to have a good idea of how the \( t\rho \) approximation should behave in our differential cross section results. This step is important in order to validate the phase space that we are studying. Our hope is to improve the calculations of our model of deuteron emission in pre-equilibrium reaction.

### 5. Goal and Conclusion

Our ultimate goal is to implement a version of the Iwamoto and Harada model in the DDHMS module of the nuclear reaction code EMPIRE[11] which performs calculations of pre-equilibrium reactions within the HMS model, and then use it to analyze data of reactions of the type (p,d).

As our previous results using Iwamoto and Harada model were not satisfactory, we are analyzing the phase space of the “pick-up” reactions using an eikonal approximation. With that, we hope to get better results and to improve the Iwamoto and Harada model.

As next steps, we will investigate the relation between our transition matrix as function of the energy and of the nucleus radius. Achieving better results, we plan to implement the Iwamoto and Harada unified model with our modifications in Blann and Chadwick’s “hybrid Monte Carlo”
Figure 2. Angular distribution data of cross section for the ground state $3/2^+$ state in $^{40}\text{Ca}(p,d)^{39}\text{Ca}$. The dots are the experimental values from Ref.[13] and the line are the predictions of the DWBA theory calculated using DWUCK [15].

model, to obtain a more physically-motivated description of pre-equilibrium deuteron emission. Inserting this result in the nuclear reactions code EMPIRE, we hope to improve the analysis of $(p,d)$ reaction data.

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