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A Short Introduction to Spallation Reactions

Theoretical Tools: Foundations and Domain of Validity

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Abstract Spallation reactions, as well as the standard theoretical tool for their study, namely the intra-nuclear cascade (INC) + evaporation model, are briefly introduced. The theoretical foundations and the domain of validity of the INC model are discussed in some detail.

1 Introduction

The name "spallation reactions" refers in general to a high-energy hadron-nucleus reaction in the ∼200 MeV to ∼3 GeV incident energy range.[1] This specification of the energy range makes the definition more oriented towards the results of the reactions, which are sketched below, rather than on a particular reaction mechanism. We will actually argue in this paper that the reaction mechanism which prevails in the above-mentioned energy range does not change really when the incident energy decreases from 200 MeV down to a few tens of MeV. Likewise, the reaction mechanism does not really change either when the incident energy goes over the 3 GeV limit, as discussed in another presentation to this conference [1]. In Sect. 2 we will shortly review the properties of spallation reactions, in particular those that are important for technological applications, which, in turn, have largely contributed to the revived interest in these reactions. In Sect. 3, the standard theoretical tool, namely the intra-nuclear cascade (INC) + evaporation model is briefly introduced. The foundations of this empirical model are discussed in Sect. 4, in connection with transport theories. In Sect. 5, the most important assumptions of both INC and transport theories are examined. Section 6 contains our conclusion.

2 Properties of the Spallation Reactions

The main property of the spallation reactions is a copious emission of light particles, mostly neutrons. The neutron multiplicity distribution for a typical case is shown in Fig. 1. On the average, about 15 neutrons are emitted. Light charged particles (protons, deuterons, tritons, etc.) and pions are also produced, at smaller (typically by an order of magnitude) rates. As a result, the target residue may be substantially lighter than the original target nucleus.

This main property is enhanced when a high-energy proton beam hits a macroscopic piece of heavy metal, a so-called spallation source. The interaction process can be viewed as an iteration of microscopic spallation

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[1] By extension, reactions induced by light nuclei with a kinetic energy per nucleon in the same energy range, are also denoted as "spallation reactions".

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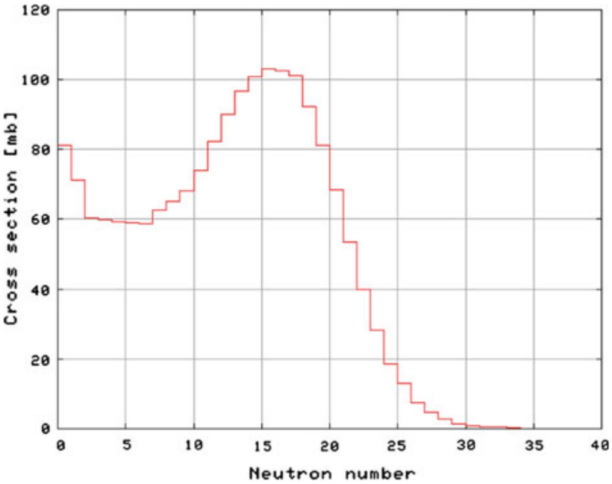

Fig. 1 Cross sections for the production of n neutrons as a function of the neutron number n in 1 GeV proton-induced reactions on Pb nuclei. Adapted from Ref. [2]

reactions.[2] Due to secondary reactions, the number of neutrons escaping from the spallation source per incident proton is higher than in a microscopic spallation reaction (or equivalently on a thin target): it may reach a few tens. On the contrary, produced charge particles are largely stopped inside the spallation source. Neutron spallation sources are used since a long time for material studies and for generation of rare and/or radioactive isotope beams. They are also intensively studied for the possible transmutation of nuclear waste in Accelerator-Driven Systems (ADS). In those future devices, a spallation source is located inside the subcritical core of a dedicated reactor, which is partially loaded with nuclear waste, containing long-lived isotopes. The neutrons issued from the spallation source multiply in the subcritical core and eventually transmute the nuclear waste (e.g. by fission for minor actinides). The first project of this kind, the MYRRHA project, has recently been launched in Belgium [3].

Although spallation sources constitute a far more expansive way of producing neutron beams than an ordinary reactor, they offer two big advantages. First the neutron source can be switched off almost instantaneously, which is important in ADS for security reasons. Second, the source may be pulsed easily, which is important for material (and other) studies. It should be noted also that, for spallation sources of standard size, the number of produced neutrons per incident proton divided by the energy of the proton beam, which is inversely proportional to the (energy) prize of a produced neutron, presents a maximum in the 1–2 GeV region [4]. This is at the origin of the standard definition of the spallation reactions mentioned in Sect. 1.

Spallation reactions are also relevant in hadrontherapy [5], in radiation protection in space missions [6] and in the study of the interaction of Galactic cosmic rays with the atmosphere [7].

3 The Standard Theoretical Tool

Serber [9] was the first to suggest that the interaction of a nucleon with energy above 200 MeV with a nucleus consists in two stages: in the first (short) one, the incident nucleon initiates a set of nucleon–nucleon collisions which emit high-energy particles and in the second stage, the target remnant loses its residual excitation energy by an evaporation-like process, emitting low-energy particles. The first stage is usually handled by the INC model. There are several models of this type on the market. We will refer here to the model developed at the University of Liège and denoted INCL, which has been proved as one of the most performing models [10]. The standard version of this model is described in Ref. [11] and the most recent version, in Ref. [12]. It is

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[2] The word "spallation reaction" or simply "spallation" is also used to designate the interaction of a high-energy particle with a macroscopic body and also refers to the ejection of many particles, mainly neutrons. The concept of macroscopic spallation reaction seems to have been introduced by Glen Seaborg in his PhD thesis on inelastic neutron scattering [8] as soon as 1937. The name "spallation" seems to have been invented by Seaborg himself, in 1947, after the much older word "spal", which designates a chip or a small piece that comes off a large piece of matter after an impact. The word "spallation" has since be used outside nuclear research, for instance in solid mechanics (flat plate impact tests), in laser application, in geology (impacts of meteorites), etc.

sufficient here to remind the salient features of the model. The INCL4 model is a simulation time-like model, which follows the fate of all particles in space-time. Particles follow straight-line trajectories, until either two of them reach a sufficiently small minimum distance of approach,[3] in which case a collision is realized, or until a particle hits the nuclear surface, in which case it is either reflected or transmitted according to transmission probability on the nuclear potential surface, or until a particle (e.g. a Δ resonance) decays. Collisions can be elastic or inelastic. Nucleon–nucleon inelastic collisions are modelized by explicitly introducing pion and Delta degrees of freedom. The final states in elementary collisions are determined at random, taking account of conservation laws and using experimental cross sections and angular distributions. Target nucleons are moving in a nuclear potential well and collisions are subject to Pauli blocking. At the end of the cascade, which is determined self-consistently (a unique feature of INCL4), an excited but largely equilibrated remnant is assumed to de-excite by evaporation/fission. Although this point is of minor interest here, we want to mention that INCL4, coupled to the evaporation-fission model ABLA07 [13], is able to give a very good description of the available spallation data (multiplicities, double differential cross sections, residue mass spectrum, residue recoil velocity, etc.) for incident energy between 200 MeV and 3 GeV. Details can be found in Ref. [14] and in the contributions of Drs. Boudard and Mancusi to this meeting [15,16].

The INCL4 model, like all INC models, uses classical trajectories, but nevertheless embodies some quantum effects: randomness in the determination of the final states of the elementary collisions, Pauli blocking applied to these final states, transmission through or reflection on the nuclear surface, average nuclear field.

4 The Theoretical Foundations of the INC Model

INC models differ in details, sometimes importantly, but they share the basic description of the interaction process as resulting from a succession of well-separated collisions, both in space and time. We will thus speak generically, in this section, of *the* cascade (or INC) model. This model may appear as a very crude, ad hoc, model, whose success is perhaps accidental. We want to argue here that the INC model possesses some theoretical foundations. The latter are provided by the so-called nuclear transport theories. These theories focus on the time evolution of quantities carrying reduced information, compared to the full wave function or the full density matrix. These quantities may be as simple as average and variance of nucleon momentum distribution. For instance, this point was investigated in detail by Pirner and his collaborators [17] in heavy-ion collisions in the GeV range. More sophisticated transport theories center on the evolution of the Wigner transform of the one-body distribution function $f(\mathbf{r}, \mathbf{p}, t)$, which can be roughly viewed as the nucleon distribution in phase space. Either starting from the Green functions formalism [18], or from the von Neumann equation [19,20], these theories arrive more or less at the same evolution equation, namely[4]

$$\left(\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m}.\nabla - \nabla U.\nabla_p\right) f = \pi\hbar^2 \int \frac{d^3p_2}{(2\pi)^3} \int \frac{d^3p_3}{(2\pi)^3} \int \frac{d^3p_4}{(2\pi)^3} |G(12 \to 34)|^2 \\ \times \{f_3 f_4 (1-f)(1-f_2) - f f_2 (1-f_3)(1-f_4)\} \delta^3(\mathbf{p}) \delta(e(p)), \qquad (1)$$

where $f_i = f(\mathbf{r}, \mathbf{p}_i, t)$. In this equation, U is the nuclear mean field, determined by the distribution f itself, G is a medium-corrected transition matrix for the nucleon–nucleon collisions and the delta functions stand symbolically for momentum and energy conservation in collisions. In the simplest approximation, U is given by

$$U(\mathbf{r}) = \int d^3\mathbf{r}' \int d^3\mathbf{p}' \langle \mathbf{r}\mathbf{r}' | G | \mathbf{r}\mathbf{r}' \rangle f(\mathbf{r}', \mathbf{p}', t). \qquad (2)$$

The transport equation is obtained after use of three main assumptions:

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[3] Less than the squared root of the total elementary cross section, divided by π.

[4] We have neglected, for pedagogical reasons, the momentum dependence of the mean field U and the retardation effects. They are not really important for the discussion of the conditions of validity.

1. *closure approximation*: the two-body correlations are unimportant in the collision term.
2. *low-gradient approximation*: for this approximation to be valid, it is required, in particular, that the mean potential U is a smooth function on the spatial extension of f, or more or less equivalently on the spatial extension of the particle wave functions.
3. *independence of collisions*: this means that, in an elementary collision, the scattering wave function becomes asymptotic before the next collision takes place.

Equation 1 has the classical form of a transport equation with a drift term (lhs) and a collision term (rhs). It is then tempting to solve this equation by simulations. This is an exact method for the drift term and it has been shown that the INC procedure provides an exact handling of the collision term, for the average (over events) one-body distribution [21,22]. One has, however, to keep in mind that the INC model is doing more than solving Eq. 1. First, in INC, the collisions are determined by the correlated two-body distribution function (in the initial state of the collisions) instead of the product of the two one-body distribution functions. In other words, the closure approximation is not made in INC, since at a given time, the distribution of the pairs of nucleons is obviously influenced by the previous collisions. Second, two-body, three-body and so on distribution functions are automatically generated in INC and are propagated under the influence of the collisions. This enables INC to predict exclusive distribution quantities (whether the INC evolution of these higher-order distribution functions is totally consistent with the higher-order transport equations besides Eq. 1 is an open question). Third, INC has the capacity to predict fluctuations, which can be compared with measured event-by-event fluctuations. There is no theoretical arguments which ensure that these fluctuations are correctly given by INC, although this seems reasonably the case in practice. To be complete, it should be emphasized that INC is certainly inferior to Eq. 1 in the treatment of the mean field U. Without entering the detail, U is considered as a fixed quantity in INC, whereas it is a function of the instantaneous distribution f in the transport equation (Eq. 2).

5 The Validity of the INC Model

5.1 A Priori Conditions of Validity

We now examine the conditions of validity of INC in parallel with those of the transport equation 1. The most important assumption common to both approaches is the dominance of independent binary collisions. Usually it is considered that this assumption is satisfied if the following conditions are met[5]

$$\pi \lambdabar_B \ll r_s \lesssim d, \tag{3}$$

where $\lambdabar_B$ is the (reduced) de Broglie wavelength for the relative motion in the entrance channel (for binary collisions), r_s is the scattering "length", i.e. the length over which the scattering wave is different from its asymptotic form and d is the average distance between a nucleon and its nearest neighbours. The first inequality in Eq. 3 has a twofold reason in INC: it guarantees that classical motion may be used and it ensures that collisions are dominant. It is often said that, under this condition, the incoming nucleon "sees" the nucleons individually. Note that, strictly speaking, for that purpose, it is sufficient that $\pi \lambdabar_B \lesssim r_s$ in INC, since the latter uses differential cross sections or probabilities for asymptotic properties (in constrast with the so-called molecular dynamics which relies on fully detailed trajectories). In addition r_s may be different from the range of the interaction potential. The sign $\ll$ is, however, necessary to legitimate the use of classical trajectories between collisions. One may argue that the derivation of Eq. 1 does not require explicitly the condition for validity of classical motion. Actually, the latter is hidden beyond the low-gradient approximation: if the extension of the particle wave functions is smaller than the characteristic variation length of the potential U, quantum motion effects are reduced. As a matter of fact, the constant $\hbar$ does not appear in the drift term of Eq. 1. It appears in the collision term because quantum transition probabilities enter this term. The quasi-absence of quantum motion effects in the nuclear transport case has been verified, at least at low energy by comparing the results for the Vlassov (classical) and the time-dependent Hartree-Fock (quantum) equations [24,25].

A delicate point deals with the role of the momentum transfer in binary collisions. General theory of scattering by a system of particles tells that if the momentum transfer q is small, the successive collisions add coherently. Therefore, soft collisions, with small q, should contribute to a coherent process. So it is tempting

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[5] The first term in Eq. 3 stands for the minimum size of the wave packet for a nucleon. It is certainly larger than $\lambdabar_B$, but many authors claim that λ_B is a more realistic value [23]. We make here a rather conservative, intermediate, choice.

to identify the latter as partly described by the mean field. These soft collisions should then be eliminated from the collision term. Unfortunately, there is no theoretical indication on how to separate large and small momentum transfer effects (see, however, an interesting discussion in Ref. [21]). In INCL4, soft collisions, defined by a maximum c.m. energy of 34 MeV, are discarded from the collision term. However, most of the time, these soft collisions are already strongly suppressed by the Pauli blocking. Another delicate point deals with the role of the mean free path. This quantity is related to the strength of the interaction and not only to the geometrical properties of the system. In a dilute and weakly interacting system, where collisions are dominant (see, however, the remark below), this quantity is related to the elementary cross section σ by

$$\lambda = \frac{1}{\rho\sigma}. \tag{4}$$

This is the average distance for a particle to make a collision or the average distance between two successive scatterings. It is then natural to require

$$r_s \lesssim \lambda \tag{5}$$

for INC to be valid. This is at variance with the second inequality in Eq. 3. Actually, condition (5) is more relevant in the strong coupling case, in particular, when λ is smaller than d. In the weak coupling case, condition (Eq. 3, second part) is more relevant, except when the coupling is so weak for λ, given by Eq. 4, to be substantially larger than d. Then, condition (5) is more relevant.

The size of the system (or the nuclear radius R in our case) does not play an important role for our discussion. If this dimension is substantially larger than λ, one can consider that particles will be emitted after many collisions. One may wonder whether INC can remain valid even if condition (Eq. 3, 2d inequality) is violated and whether the possible interferences between the different paths may cancel out. If the size of the system is smaller than λ, the interaction basically reduces to a single collision and, a priori, INC is well suited to the case.

5.2 Analysis of the Effective Validity of the INC

To see whether condition (3) (or (5)) is realized for a given system, it is convenient to look at Fig. 2. Therein are compared different characteristic lengths. The red slashed curve gives the de Broglie wavelength of the incoming nucleon, multiplied by π. The horizontal arrows indicate the radius of a typical heavy nucleus R, and the quantities d and r_s defined above, respectively. The latter quantity is not well known. It is believed to be of the order of 1 fm at least. From Fig. 2, it can be seen that condition (3) is realized (marginally) for $E_{lab} \gtrsim 200$ MeV. The conditions of validity of INC seem to be realized between 200 MeV and a few GeV. The upper limit corresponds to the excitation of the internal nucleon degrees of freedom,[6] signalled by the success of string models like PYTHIA [26]. There is no worry about which one of conditions ($r_s \lesssim d$) and ($r_s \lesssim \lambda$) should prevail, since, in this energy range, the mean free path is approximately equal to the distance d.

One has to realize that, at 200 MeV, condition (3) is barely fulfilled only, and for the first collision only. Subsequent collisions happen at lower and lower energy and the validity of INC is less and less ensured. In spite of this unfavourable conditions, the INC model (and INCL4 in particular) continues to give rather satisfactory results with decreasing incident energy below 200 MeV, with, however, a decreasing agreement [10,27,28]. We give two examples in Fig. 3. So, the question arises to know why INC is working well in conditions where it should not, a priori. There is no satisfactory answer to this question, up to now. Elements can be found in Fig. 2 and in the transport theory. When the energy is going down from 200 to ∼40 MeV, the de Broglie wavelength is becoming larger than r_s, that is considered approximately equal to the range of the interacting potential. One is facing the scattering of a wave packet with a size of $\sim \pi \lambdabar_B$ by a potential with range r_s. As far as the "scattering length" is concerned, the effective value of the latter is roughly speaking equal to $r_s^{eff} \approx r_s + \pi \lambdabar_B$. At the same time, due to Pauli blocking, the mean free path is no more equal to expression (4), but becomes substantially larger. One has thus $r_s^{eff} < \lambda$, which replaces the last inequality of Eq. 3. The first inequality of Eq. 3 is less and less fulfilled, but this does not matter so much, since the collision term in Eq. 1 does not require this condition (only the independence of collisions is necessary). Of course, at some

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[6] The opening of other hadronic degrees of freedom, indicated by the thresholds of pion and nucleon–antinucleon productions in Fig. 2 (vertical arrows), does not pose any problem, since these degrees of freedom are similar to nucleon ones. Simply, Eq. 1 is generalized to a set of coupled similar equations.

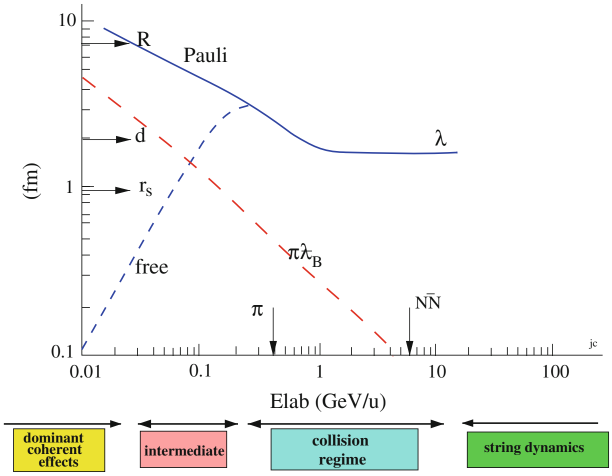

Fig. 2 Comparison of various characteristic lengths of a nucleon-nucleus system as functions of the incident kinetic energy E_{lab}. The *blue curves* correspond to the mean free path, as calculated by Eq. 4, with ρ equal to the normal nuclear matter density, taking account of the Pauli blocking (*full line*) or not (*dotted line*). See text for detail

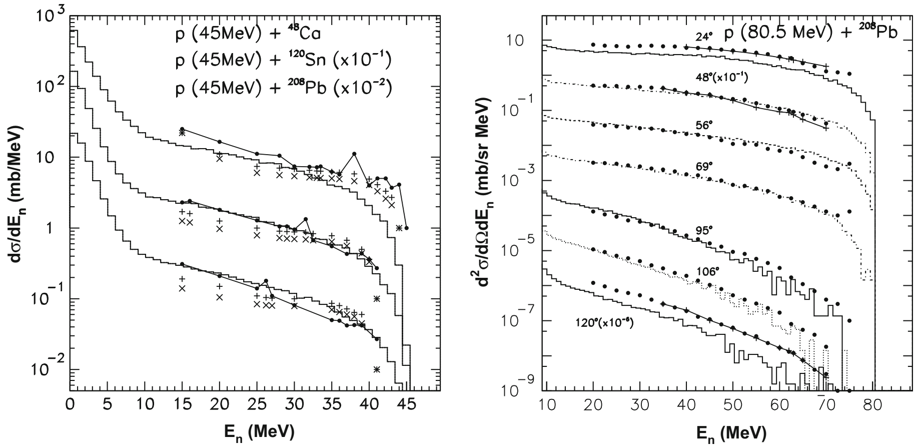

Fig. 3 *Left panel* energy differential cross-section for neutron production in proton-induced reactions on three targets at 45 MeV incident energy. Data (*dots*, with an accuracy of about 20%) are taken from Ref. [29] and are compared with the predictions of INCL model (*histograms*). The × and + symbols are the results of pre-equilibrium models. See Ref. [28] for detail. *Right panel* double differential neutron cross-sections for proton-induced reactions on ^{208}Pb at 80.5 MeV. Data (*dots*, with an uncertainty of about 20%) are taken from Ref. [30]. For the sake of clarity, the double differential cross-sections are displayed after multiplication by 10^0, 10^{-1}, 10^{-2}, etc., for angles in increasing order. Data are compared with the predictions of INCL model (*histograms*). Figure adapted from Ref. [28]

small enough value of the incident energy, typically 40–50 MeV, the size of the wave packet is sufficiently large to imply two target nucleons at the same time, with a large probability, and the cascade picture breaks down. In other words, at the low energy range under discussion, the collisions are becoming less numerous but remain independent. The wave packets describing the nucleons are becoming larger, but the collision rate is not really dependent upon the details of the nucleon motion since it is determined by the flux of particles (the f-distribution), as this is embodied by the transport equation. The validity of INC at low energy may be reinforced by the observation that half of the total reaction cross section corresponds to impact parameters that are beyond the half density radius. For these impact parameters, the interaction practically reduces to one collision, for which INC is anyway well suited. For the other impact parameters, the reaction is more central and only one or two collisions are sufficient to absorb the incoming nucleon. So, one half of the events lead to a "thermalized" compound nucleus with a large probability and for the other half, the incoming nucleon sees a low-density region. In both cases, INC is well suited. This last argument, admittedly crude, is developed in Ref. [31].

6 Conclusion

We have shortly presented the spallation reactions, as well as the standard theoretical tool, the INC+evaporation model, for studying these reactions. We have motivated the rather empirical INC model by nuclear transport theory. We have examined the conditions of validity of the INC model and verified that they are fulfilled for incident kinetic larger than 200 MeV. We have given tentatively a circumstantial explanation of the success of the model below 200 MeV.

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