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PRE-EQUILIBRIUM PROCESSES IN NUCLEAR REACTIONS: INTERCOMPARISON OF THEORIES AND CODES

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Abstract: The present status of the theories and the associated computer codes that are used to calculate the cross-sections of pre-equilibrium processes in nuclear reactions is reviewed. The principal theories used at the present time are the varieties of exciton models and the quantum-mechanical theories. The codes used to calculate the direct interaction and compound nucleus cross-sections are also mentioned.

1. Introduction

In recent years there have been many studies of multistep processes in nuclear reactions partly because of their importance for a full understanding of the reaction mechanism and partly for their application to fusion reactor design. It is now clear that multistep processes make large contributions to the cross-sections of the reactions of 14 MeV neutrons that take place when the neutrons from the $d-t$ fusion reaction enter the surrounding material. It is necessary to choose this material to minimise the production of unwanted radio-activity and to maintain its structural rigidity in spite of the intense neutron bombardment to which it is subjected. This latter requirement implies the minimisation of proton and alpha-particle emitting reactions, since these can ultimately give rise to bubbles of hydrogen and helium that weaken the material. Although many of the required cross-sections have been measured, and these measurements are indeed essential to test theories of nuclear reactions, it is not possible to measure all the cross-sections that are required by reactor designers. Very many cross-sections are required, and it would be exceedingly costly and laborious to measure them all. Furthermore, the reaction flux is so intense that secondary and even tertiary reactions can occur with unstable nuclei resulting from the primary interactions, and these are impossible to measure. What is therefore required is a fast yet sufficiently accurate way of calculating the needed cross-sections, and this in turn can only come from a thorough understanding of the mechanism of the reactions.

The theory of nuclear reactions has developed over the last sixty years, and now it is possible to describe them in some detail. In this review we are primarily concerned with the interactions of nucleons from about 10 to 100 MeV. Proton reactions are included as well as neutron reactions because it is often easier to obtain their cross-sections experimentally and the resulting data is valuable to test the accuracy of reaction theories and to determine the values of their parameters.

Nuclear reactions take place in a series of stages corresponding to the successive interactions of the incident particle with the nucleons of the target nucleus. At each stage energy may be given to the target nucleons, until ultimately the energy of the projectiles is shared statistically among them. The first stage in this process takes place in a time similar to the transit time, generally around 10^{-22} to 10^{-23}s. When the incident energy is distributed among the target nucleons an excited compound system is formed which can subsequently decay by particle emission, followed by gamma emission, until it reaches a ground state. The decay of the compound nucleus takes place over a much longer time-scale, typically about 10^{-16}s. For many years it was considered sufficient to divide the nuclear reaction process into these two stages, the direct stage and the compound nucleus stage. The cross-sections of the direct processes can be calculated by direct interaction theories and those of the compound nucleus reactions by the Weisskopf-Ewing or Hauser-Feshbach theories, and then added to obtain the complete cross-section.

Many studies have now shown that this division into two stages is inadequate; there is definite evidence that particles can be emitted after the first direct interaction but long before the attainment of statistical equilibrium; they are referred to as the pre-equilibrium particles.

This evidence came in many forms. Principally it proved impossible to fit some of the measured energy and angular distributions of the emitted particles by a combination of direct interaction and compound nucleus theories. Some cross-sections were found, for example, that are symmetric about 90°, attesting to their compound nature, and yet they contained far more energetic particles than could be accounted for by statistical emission from a fully equilibrated nucleus. Conclusive evidence for pre-equilibrium emission was provided by analyses of the fluctuations of excitation functions, which provided estimates of the lifetimes of the intermediate states.

The first models of pre-equilibrium emission were semi-classical in nature, and provided a simple means of calculating the energy distributions of the emerging particles, using parametrised expressions for the interaction matrix elements. Subsequently these models were extended to give the angular distribution as well. In more recent years fully quantum-mechanical theories have been developed that provide, at least in principle, a parameter-free method of calculating the required cross-sections.

In this review, the essentials of the exciton model and quantum mechanical theories are summarised in sections 2 and 3, and some computer programs that are being used for practical calculations are discussed in section 4. Particular attention is paid to the problems of assessing their reliability and usefulness, not only for analysing measured cross-sections but also for predicting unknown ones. It is not of course possible to give here a full account of the formalism of these theories, so frequent reference is made to the original publications where this may be found. Some conclusions are given in section 5.

2. The Semi-Classical Models.

Since the basic work of Griffin in 1966[1], a variety of different pre-equilibrium models has been developed; see reviews by Blann 1975; Gadioli *et al* 1976, 1980; Bunakov 1978[2]. The most widely used models are the intranuclear cascade model (INC), the Harp-Miller-Berne[3] (HMB) model and, particularly, the exciton (EM) and the geometry-dependent hybrid (GDH) models.

A classical approach to precompound decay is provided by the INC-model (Chen *et al* 1968; Bertini *et al* 1974)[4]. The trajectories of the particles inside the nucleus are followed in coordinate space by means of Monte-Carlo methods. The numerical simulation of the scattering process is based on experimental free nucleon-nucleon scattering cross-sections and angular distributions. Up to 1975 the INC-model was the only pre-equilibrium model able to predict angular distributions of emitted particles. However, the emission into the backward hemisphere is underestimated by several orders of magnitude.

In the HMB-model (Harp, Miller and Berne, 1968)[3] the energy scale is divided in bins and the average number of occupied single-particle levels in each bin is computed, usually in the framework of the Fermi-gas model. The occupation of nucleons in each bin changes in time due to the intranuclear collisions. The evolution of this excited nuclear Fermi gas is followed through numerical computation of the relative occupation of each bin as a function of time by solving a set of coupled differential equations (Boltzmann-like transport equations). The transition rates are obtained from experimental free nucleon-nucleon scattering cross-sections. In contrast to the INC-model, this model permits a quantum-statistical treatment, although in practice the transition rates are computed in a classical manner. However, it cannot predict angular distributions. Another practical disadvantage of the HMB-model is its computational complexity. To overcome this difficulty, additional assumptions have to be introduced. This is done in the exciton and hybrid models, which have become the most popular pre-equilibrium models for applications in nuclear data evaluation.

The EM- and GDH-models, originating from the work of Griffin[1], are closely related. In these models the nuclear state is characterized by the excitation energy E and the total number n of particles p above and holes h below the Fermi surface. Furthermore, in the EM it is assumed that all possible ways of sharing the excitation energy between different particle-hole configurations with the same exciton number n have equal *a-priori* probability. Instead of tracing the evolution of the occupation of each energy bin, as in the HMB-model, one merely traces the temporal development of the exciton number n, which changes in time as a result of intranuclear collisions. This assumption makes pre-equilibrium theory amenable for practical calculations. The price to be paid is the introduction of an assumption of *a-priori* equal probabilities, so that for the transition rates some effective average is taken over all possible configurations of the nucleus. The average transition-matrix element is parametrized as a function of energy and mass.

In the hybrid model an attempt is made to retain some more elements from the HMB-model, e.g. by relating the internal transition rates to the free nucleon-nucleon scattering cross-section, using the concept of mean free path in nuclear matter. A further refinement has been made in the geometry-dependent hybrid model (GDH) by taking into account the variation of nuclear density at the nuclear surface (Blann[2]).

2.1 Spin-independent exciton model

In EM the differential cross section is denoted by

$$\frac{d\sigma}{d\epsilon}(a,b) = \sigma_a \sum_{\substack{n \\ \Delta n=2}} W_b(n,\epsilon)\tau(n), \qquad (2.1)$$

where σ_a is the composite-formation cross-section, W_b is the emission rate and τ is the mean life time. The summation is performed over all possible exciton states n, starting with the initial number n_0 equal to 3 for nucleon-induced reactions. The emission rate of particle b is calculated from

$$W_b(n,\epsilon) = \frac{2s_b+1}{\pi^2\hbar^3}\mu_b\epsilon\sigma_b^{inv}(\epsilon)\frac{\omega(p-p_b,h,U)}{\omega(p,h,E)}Q_b(n), \qquad (2.2)$$

where s_b, μ_b, σ_b^{inv} are the spin, reduced mass and inverse-reaction cross-section referring to particle b, respectively. The state density ω is calculated from the well-known Williams[5] formula with or without pairing and other corrections. In eq.(2.2) p_b denotes the number of nucleons in particle b, U is the residual energy, E is the initial energy and $Q_b(n)$ is a factor (Cline[6]) enhancing the emission of ejectiles of type a at the lowest exciton numbers so as to account for the "memory of the projectile by the nucleus" in the first stages of the reaction; $Q_b(n) \to 1$ for large values of n (Kalbach[7]). The mean lifetime of exciton state n follows from the time-integrated master equation:

$$\begin{aligned} -q_0(n) = {} & \lambda^+(n-2)\tau(n-2) + \lambda^-(n+2)\tau(n+2) \\ & - [W_t(n) + \lambda^+(n) + \lambda^-(n)]\tau(n), \end{aligned} \qquad (2.3)$$

where $q_0(n)$ is the initial exciton distribution, taken as δ_{nn_0} for first emission, $\lambda^{\pm}$ are the internal transition rates and $W_t(n)$ is the total emission rate obtained by integrating $W_b(n,\epsilon)$ over all outgoing energies and summing over all outgoing particles. For the internal transition rates the simplest expressions are (Williams[5]):

$$\lambda^+(n) = \frac{2\pi}{\hbar} < M^2 > g^3E^2/(n+1), \qquad (2.4a)$$

$$\lambda^-(n) = \frac{2\pi}{\hbar} < M^2 > gph(n-2), \qquad (2.4b)$$

where $< M^2 >$ is an average residual matrix element, that is often parametrized as follows (Kalbach[7]):

$$< M^2 >= CA^{-3}E^{-1}. \qquad (2.5)$$

In practice more complicated expressions and parametrizations (Kalbach[8]) are sometimes used. It is also possible to relate $< M^2 >$ to the nucleon-nucleon mean free path in nuclear matter. One of the most fundamental questions of EM is whether all relevant internal transitions can be written in the form of an expression like (2.4), by averaging over all possible configurations of the nucleus.

In the STAPRE program (Strohmaier and Uhl[10]) a random-walk equation (Akkermans and Gruppelaar[11]) is followed rather than eq.(2.3). Under plausible assumptions this is mathematically equivalent to the master-equation approach (Akkermans[12]). Both approaches also comprise the equilibrium or evaporative stage of the re-

action. The EM is basically an exclusive model, but it may be extended (like the Hauser-Feshbach model) to multi-particle emission. In multi-particle emission precompound effects in secondary emission are only important at energies above about 25 MeV (Akkermans and Gruppelaar[11]). Similar equations apply, assuming that in (2.3) the initial distribution is calculated from the previous stage.

The neutron spectra from the ^{93}Nb(n,n') reaction at 7, 9 12.3 and 14.6 MeV have been analysed using the program STAPRE by Mittag *et al*[13]. They found that the single-particle exciton model is not able to account for the higher-energy emitted particles over the whole range of incident energies, and that it is necessary to include a collective excitation component that can be evaluated by direct reaction theory.

2.2 Spin-dependent exciton model

In Hauser-Feshbach codes (HF) the summation in eq.(2.1) is usually limited to the equilibrium exciton number $\bar{n}$ and λ^- is set equal to zero in eq.(2.3). This "never-come-back" approximation leads to the closed-form expression:

$$\frac{d\sigma^{\text{preq}}}{d\epsilon}(a,b) = \sigma_a \sum_{\substack{n=n_0 \\ \Delta n=2}}^{\bar{n}} W_b(n,\epsilon)\frac{1}{\Lambda(n)} \prod_{\substack{m=n_0 \\ \Delta m=2}}^{n-2} \frac{\lambda^+(m)}{\Lambda(m)}, \tag{2.6}$$

where the product represents the "depletion" factor D_n namely the fraction of nuclei that have not yet emitted a particle and where $\Lambda(n) = W_t(n) + \lambda^+(n)$ is the total escape rate. In modified HF codes the following substitution is made:

$$\frac{d\sigma}{d\epsilon}(a,b) = \{1 - f^{\text{preq}}\}\frac{d\sigma^{HF}}{d\epsilon}(a,b) + \frac{d\sigma^{\text{preq}}}{d\epsilon}(a,b), \tag{2.7}$$

with f^{preq} equal to the preequilibrium fraction, defined by the ratio of (2.6) to (2.1).

The main advantage of (2.7) is that in the equilibrium part the spin- and parity-selection rules are still obeyed. For further (multi-particle) emission the spin-parity population of the preequilibrium part is usually taken from the equilibrium model.

In recent work it has been attempted to include spin and parity[14,15] in (2.1–2.4). Formally this "unified" or "consistent" model can be represented by:

$$\frac{d\sigma}{d\epsilon}(a,b) = \sigma_a \sum_{J_\pi}\sum_{n} W_b^{J_\pi}(n,\epsilon)\tau^{J_\pi}(n) \tag{2.8a}$$

or

$$\frac{d\sigma}{d\epsilon}(a,b) = \sigma_a \sum_{J_\pi} q_0^{J_\pi}(n_0)\frac{\sum_n W_b^{J_\pi}(n,\epsilon)\tau^{J_\pi}(n)}{\sum_n W_t^{J_\pi}(n)\tau^{J_\pi}(n)}, \tag{2.8b}$$

where τ^{J_π} is the solution of a master equation like (2.3) with all quantities indexed by the spin J and parity π of the composite state and with initial condition $q_0^{J_\pi}(n_0) = \sigma_a^{J_\pi}/\sigma_a$.

At equilibrium eq.(2.8) coincides with the HF expression. The main problem is to calculate τ^{J_π} without a sound knowledge of the spin-dependence of $\lambda_+^{J_\pi}$. Therefore, approximate solutions have been suggested by assuming in (2.8b):

$$\tau^{J_\pi}(n) = s^{J_\pi}(n)\tau(n), \tag{2.9}$$

with s^{J_π} independent of n (Gruppelaar[15,16]) or proportional to the n-dependent spin distribution of the level density (in the TNG code of Fu[19]). In PERINNI (Sect.4) s^{J_π} as well as the spin distribution of the level density are assumed to be independent of n, which is rather too simple. The use of eq.(2.8) leads to different composite-particle emission cross-sections (Bisplinghoff[17]) and to different spin-populations compared to eq.(2.7), of importance in multi-particle emission. There are indications that the constant spin-parity population assumption is most realistic (Gruppelaar[15]).

2.3 Angular distributions

At high values of $n(> \bar{n})$ the random-phase approximation holds (Plyuiko[18]); on the other hand, completely correlated phases are expected at the initial $n = 0$ stage (Fu[19]). By introducing an n-dependent factor, indicating the fraction of the angular-distribution calculated according to the fully-correlated phases, Fu[19] was able to obtain satisfactory fits to angular distributions of inelastically scattered neutrons at $E = 14$ MeV ("generalized HF-theory"). Earlier, Plyuiko[18] has adopted the random-phase approximation at all values of n.

The most important contribution to the precompound angular distribution in inelastic neutron-scattering comes from the $n_0 = 3$ component, that corresponds at sufficiently high incident energies to a single collision. This offers the possibility of calculating the angular distribution in a rigorous way for particles emitted after just one collision, using the Kikuchi-Kawai (KK) expression[20] for scattering in nuclear matter (Costa *et al*[21], Blann *et al*[22]). Representing the double-differential cross-section by:

$$\frac{d^2\sigma(a,b)}{d\epsilon d\Omega} = \sigma_a \sum_n W_b(n,\epsilon)\tau(n)\sum_\ell \frac{2\ell+1}{4\pi} f_\ell(n) P_\ell(\cos\theta), \tag{2.10}$$

it is found (Costa *et al*[21]) that:

$$f_1(3) = \xi_1(E,\epsilon), \tag{2.11}$$

where ξ_1 is the reduced Legendre coefficient of the KK angular distribution. For higher values of n the energy information of particles is no longer available in the exciton model. Therefore an energy-averaged KK-kernel (Ziyang *et al*[23]) has been suggested by Costa *et al*[21] to calculate the Legendre coefficients at higher values of n. This is possible with the "generalized exciton model" of Mantzouranis *et al*[24], e.g. in the mathematical formulation of Akkermans[25]. An extension of this model has been made by Iwamoto and Harada[26]. Effects of refraction are important at low incident and outgoing energies (Gruppelaar and Akkermans[27]). A classical estimate of these effects has been made by Costa *et al*[21]. Finite-size effects are accounted for by truncating the angular distribution. The results agree with the systematics of Kalbach and Mann[28]. Further refinements are possible by accounting for a finite nuclear temperature rather than the zero-temperature Fermi distributions used by KK (De *et al*[29]).

Extensive calculations of neutron reaction cross sections in the energy range 20–100 MeV have been made by the Los Alamos group[30] using the one-component exciton model of Kalbach[31]. In this model the excitation energy available to a hole is limited by the assumption of a shallower depth of the nuclear potential near the nucler surface, and holes with excitation energies exceeding the effective well depth are excluded from the normally calcu-

lated state densities. Correction for this effect increases the cross-section for the emission of the more energetic particles by more than a factor of two, significantly improving the agreement with the experimental data. They also included in their calculations the possibility that after pre-equilibrium particle emission the residual nucleus still has enough energy to emit further pre-equilibrium particles[32], and found that it had rather a small effect at 90 MeV but a much more important effect at 200 MeV.

2.4 Geometry-dependent hybrid models

Next, we give some expressions for the hybrid and GDH-models originating from the work of Blann[2]. The hybrid-model cross-section is calculated from the expression:

$$\frac{d\sigma^{\text{preq}}}{d\epsilon}(a,b) = \sigma_a P_b(\epsilon) = \\ = \sigma_a \sum_{\substack{n=n_0 \\ \Delta n=2}}^{n} X_n \frac{N_n(\epsilon,U)}{N_n(E)} \frac{\lambda_c(\epsilon)}{\lambda_c(\epsilon)+\lambda_+(\epsilon)} D_n, \tag{2.12}$$

which closely resembles (2.6) after substitution of (2.2). However, the meaning of the various quantities is somewhat different, partly because of different bookkeeping; see Blann and Vonach[33] for the exact definitions. Discussion of EM/(GD)H bookkeeping differences has been given by Gadioli *et al*[34], Blann[35], Akkermans[36] and Bisplinghoff[17]. One important difference is that the transition rate $\lambda_+(\epsilon)$ is a function of ϵ referring to the individual particle rather than to the nuclear system as a whole as in EM. Thus, one may say that (GD)H is an independent-particle model whereas EM represents a systems approach. Bisplinghoff[17] states that in addition EM assumes complete particle-hole configuration mixing within exciton classes, while (GD)H assumes no configuration mixing at all. The quantity $\lambda_+(\epsilon)$ is evaluated (Blann[2]) from the relation

$$\lambda_+(\epsilon) = \sqrt{\frac{2(\epsilon+V)}{m}} \bar{f}(\epsilon), \tag{2.13a}$$

where V is the real potential and $\bar{f}(\epsilon)$ is the mean free path in nuclear matter:

$$\bar{f}(\epsilon) = 1/\rho < \sigma >, \tag{2.13b}$$

in which ρ is the density of nuclear matter and $< \sigma >$ is the average effective KK cross-section for a nucleon-nucleon interaction in nuclear matter (Kikuchi and Kawai[20]). Unfortunately, the results from (2.12, 2.13) are only satisfactory when $\bar{f}(\epsilon)$ is multiplied with a factor of about 2. This situation is improved when the GDH version is used:

$$\frac{d\sigma^{\text{preq}}}{d\epsilon}(a,b) = \pi\lambda^2 \sum_{\ell} (2\ell+1) T_\ell P_b(\ell,\epsilon), \tag{2.14}$$

where $P_b(l,\epsilon)$ is defined (Blann and Vonach[33]) similar to (2.12–2.13), with however, ℓ-dependent quantities. In this way longer mean free paths are used for nucleons in the diffuse surface region, parametrized by the impact parameter ℓ. Another result of applying (2.14) is more emission at high values of ϵ, where the EM yields much lower cross sections. Attractive points of the GDH model are: no parameter adjustment needed and good predictions in a large mass and energy range.

The geometry-dependent hybrid model has been used by Ivascu *et al*[37] to calculate the (n,p), (n,α) and $(n,2n)$ excitation functions and also the neutron, proton and alpha-particle emission spectra at 14 MeV neutron energy from isotopes of Fe, Cr and Ni. The model included angular momentum and parity conservation, and gave a good account of the experimental data (see Fig.1).

The unification of pre-equilibrium models has recently been discussed by Gruppelaar and Akkermans[38], with special reference to the incorporation of angular momentum conservation and to their microscopic foundations. They show that it is possible to derive a master equation that includes angular momentum conservation, and embodies the Hauser-Feshbach and exciton models as limiting cases. This theory is suitable for practical applications and can be extended to give the cross-sections

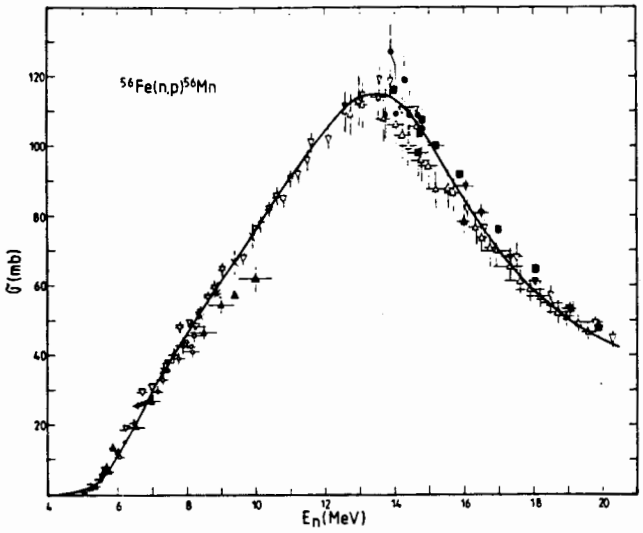

Fig.1. Total cross-section for the reaction $^{56}\text{Fe}(n,p)^{56}\text{Mn}$ as a function of neutron energy compared with geometry-dependent hybrid model calculations, including angular momentum and parity conservation (Ivascu *et al*[37]).

for the excitation of discrete states whose structure is known. It is closely related to the theory of Agassi, Weidenmüller and Mantzouranis[39] and unifies the Hauser-Feshbach, Weisskopf-Ewing and exciton models. They also discuss in some detail the extension of the master equation model to calculate angular distributions. This is quite straightforward for the multistep compound component, since this is symmetric and can be obtained by generalising the Hauser-Feshbach theory (Plyuiko[18]). It is more difficult to calculate the angular distribution for the multistep direct contribution. It is possible to insert the leading particle approach[21,25,26,40] into the spin-dependent master equation, but this has the defects of a semi-classical treatment and is difficult to justify microscopically. Another method is that of Fu, who introduces a phenomenological weighting function to connect the phases of the states in the different stages of the excitation chain[19].

3. The Quantum Mechanical Theories

Quantum-mechanical theories of pre-equilibrium reactions have been formulated by Feshbach, Kerman and Koonin[41] (see also Feshbach[42]) and by Tamura *et al*[43] and applied to analyse experimental data (Avaldi *et al*[44]; Bonetti *et al*[45,47]; Hodgson and Chadwick[46]; Herman *et al*[48]).

The Feshbach-Kerman-Koonin Theory

The basic physical picture underlying the quantum-mechanical multistep theory is the same as for the exciton model. It is assumed that the interaction between the incident nucleon and the target nucleus takes place in a number of stages of increasing complexity. To evaluate the probability of emission after the first stage but before the attainment of statistical equilibrium it is necessary to consider the mechanism of nuclear excitation in detail. The nucleus is excited by a series of nucleon-nucleon collisions between the projectile and the target nucleons. These take place in stages, or doorway states of increasing complexity beginning with the projectile in the continuum. The first interaction creates a particle-hole pair, giving a 2-particle 1-hole (2p1h) state. There are a large number of possible 2p1h states. Subsequent interactions create additional particle-hole pairs, giving 3p2h states and once again there are very many 3p-2h states for each 2p1h state. This process continues until the excitation is spread through the nucleus to produce a fully-equilibrated nucleus which then decays statistically.

At each stage it is useful to consider separately the states with at least one particle in the continuum and the states with all particles bound; these states may be formally described by the projections P and Q acting on the total waveform Ψ, with $P+Q=1$. The set of states $P\Psi$ contribute to the multistep direct process and the complementary set of states $Q\Psi$ to the multistep compound process. These states are shown in Figure 2, with the arrows indicating transitions from one configuration to another. If only two-body interactions are present these transitions can only take place between neighbouring stages; this is the chaining hypothesis.

At each stage there are three possibilities: excitation of an additional particle-hole pair, de-excitation of a particle-hole pair and emission into the continuum. The transition matrix for the de-excitation of a particle-hole pair is the same as the corresponding matrix for its excitation, but because the density of final states is so much greater for the states with more particle-hole pairs the probability of excitation of an additional particle-hole pair is much greater than that of de-excitation. Thus transitions to states of greater complexity are much more probable than transitions to states of lesser complexity. It is therefore good approximation to neglect the transitions going to states of lower exciton number; this is the never-come-back assumption.

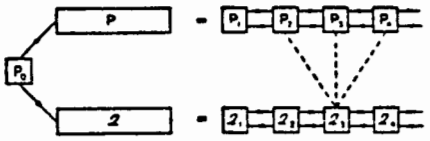

Fig.2 Multi-step description of a nuclear reaction.

The pre-equilibrium emission can take place directly at each stage from the P-chain, or indirectly from the Q chain. In the latter case the emission process goes through states in the P-chain; this can happen in three different ways as shown in Fig. 2 . The more energetic particles come from the early stages of the chain and the less energetic from the later stages.

The time structure of the interactions is more complicated. The multistep direct reactions take place down the P-chain, and these direct processes take place rapidly. The transitions down the Q-chain, on the other hand, take place much more slowly, and indeed a state of quasi-equilibrium is attained at each stage so that the emission is compound in character with a symmetric angular distribution. A large number of individual interactions take place at each stage, but nearly all of them leave the number of particles and holes unchanged. It is only very occasionally that a collision results in a transition to a state of greater complexity or to the P-chain and hence to the continuum. To obtain the emission probabilities only these escape probabilities need be calculated, together with the probabilities for exciting a further particle-hole pair. The vastly greater number of interactions taking place within each stage in the Q-chain without changing the exciton number are only important for their role in ensuring statistical equilibrium at each stage.

The relative reaction fluxes passing down the P and Q chains depends strongly on the incident energy. At low energies the Q-chain interactions dominate, giving symmetric multistep compound angular distributions. As the energy increases the P chain interactions become increasingly important until finally they are responsible for almost all the cross-section giving forward-peaked multistep direct angular distributions. The transitions between the P and Q chains are small and average out, so that the contributions of the P and Q chains can be evaluated separately, and their sum compared with experiment.

The Multistep Compound Theory.

To describe the multistep compound process mathematically, let $\Gamma_n^{\downarrow}$ be the damping width corresponding to the transition from the n^{th} to the $n+1^{\text{th}}$ state, and $\Gamma_n^{\uparrow}$ the escape width for the transition from the n^{th} state into the continuum. The total width for the decay of the n^{th} state is therefore

$$\Gamma_n = \Gamma_n^{\downarrow} + \Gamma_n^{\uparrow} \tag{3.1}$$

The total probability for emission into the continuum from the n^{th} state is then the product of three factors for each value of the total angular momentum J:

(a) the probability of formation of the compound system, which is given by the optical model expression

$$\sigma_C^{\ell J} = \pi\lambda^2 \frac{2\pi < \Gamma_{\ell J}^{in} >}{< D_{\ell J} >} \tag{3.2}$$

where the last factor is the strength function.

(b) the probability of the system arriving to the N^{th} stage without particle emission. This is given by the product of the probabilities of surviving the m^{th} stage,

$$\prod_{m=1}^{N-1} W_{m+1,m} = \prod_{m=1}^{N-1} \frac{< \Gamma_{mJ}^{\downarrow} >}{< \Gamma_{mJ} >} \tag{3.3}$$

where $< \Gamma_{mJ}^{\downarrow} >$ is the damping width for the transition to a stage of higher exciton number and $< \Gamma_{mJ} >$ is the total width.

(c) the probability that a particle will be emitted into the continuum from the N^{th} stage. This is given by a sum over all possible emission processes divided by the sum over all processes. Emission can take place in three ways, so the emission probability is given by the sum of products of emission widths $\Gamma_{NJ}^{\uparrow \ell s \nu}(U)$ and the level densities $\rho_J^N(U)$ of the final states of the residual nucleus at excitation energy U. This gives

the factor

$$\frac{\left\langle \Gamma^{\uparrow \ell s \nu}_{NJ}(U)\rho^{N}_{J}(U)\right\rangle}{<\Gamma_{NJ}>} \tag{3.4}$$

Collecting these factors together gives for the double differential cross-section for pre-equilibrium emission by the multistep compound process

$$\frac{d^2\sigma}{d\Omega d\epsilon} = \pi\lambda^2 \sum_J (2J+1)\left[\sum_{N=1}^{r}\sum_{ls\lambda\nu} C^{\lambda}_{lsJ} P_\lambda(\cos\theta) \times \sum_\nu \frac{<\Gamma^{\uparrow l e \nu}_{NJ}(U)\rho^N_J(U)>}{<\Gamma_{NJ}>}\right] \times \left(\prod_{m=1}^{N-1}\frac{<\Gamma^{\downarrow}_{mJ}>}{<\Gamma_{mJ}>}\right)\frac{2\pi <\Gamma^{in}_{\ell J}>}{<D_{\ell J}>} \tag{3.5}$$

All the factors in the above expressions are calculated quantum-mechanically or, as in the case of the level density function, obtained from the known systematics of nuclear properties. The measured cross-section for the formation of the compound nucleus is used, and if it is not available it can be obtained from the optical model.

The particle-hole level densities are calculated using Ericson's expression based on the equidistant spacing model, with an additional factor giving the spin distribution

$$\rho^N_J(E) = \rho_N(E) S^N_J \equiv \rho_n(E) S^n_J \tag{3.6}$$

where $n = 2N+1$ and

$$\rho_n(E) = \frac{g(gE)^{n-1}}{p!h!(n-1)!} \tag{3.7}$$

in which g is the total single-particle density and p, h the numbers of particles and holes ($n = p+h$).

The spin-dependent factor S^n_J is given by

$$S^n_J = \frac{2J+1}{\sqrt{\pi}\, n^{3/2}\sigma^3}\exp\left[-\frac{(J+\frac{1}{2})^2}{n\sigma^2}\right] \tag{3.8}$$

The spin cut-off parameter σ^2 is related to the nuclear temperature τ by the expression

$$\sigma^2 = 2C\tau \tag{3.9}$$

where $C \sim A^{2/3}/90$ (MeV^{-1}) and

$$E = a\tau^2 - \tau \tag{3.10}$$

and $a = \pi^2 g/6$.

Each of the widths corresponding to the three emission processes may be expressed as a product of three factors, the first depending on the level densities, the second on angular momentum coupling and the third on the wavefunctions of the interacting particles:

$$<\Gamma^{\uparrow \ell s \nu}_{NJ}(U)\rho^\nu_s(U)> = X^{\ell s \nu}_{NJ}(U) A^\nu_N(U)\theta^\nu_N(U). \tag{3.11}$$

The full expressions for the first two of these functions are given by FKK and the third is

$$\theta(U) = V_0\left(\frac{4\pi}{3}r_0^3\right)\frac{1}{4\pi}\int_0^\infty u_{j1}(r)u_{j2}(r)u_{j\ell}(r)u_{j3}(r)dr/r^2 \tag{3.12}$$

where V_0 is the strength of the residual two-body interaction and the radial wave functions $u_{j1}(r)$ and $u_{j2}(r)$ refer to the bound particles before the interaction, $u_{j3}(r)$ to the bound particle after the interaction and $u_{j\ell}(r)$ to the particle emitted into the continuum.

At lower energies where there are few contributing channels it is possible to fix the strength of the effective interaction V_0 directly and accurately by normalising the sum of the cross-sections in all the reaction channels to the total reaction cross-section σ_R obtained from the optical model potential or from experiment. Thus at a particular energy

$$\sum_i V_0^2 f_i(E) + \sum_j \sigma_j(E) = \sigma_R \tag{3.13}$$

where i, j label the reaction channels. $V_0^2 f_i(E)$ is the total reaction cross-section in the i$^{\text{th}}$ channel and $\sigma_j(E)$ that in the j$^{\text{th}}$ channel. In this expression the cross-sections in the first i channels are calculated using the multistep theory, and those in the remaining j channels are either calculated by the Weisskopf-Ewing theory or taken from experimental data.

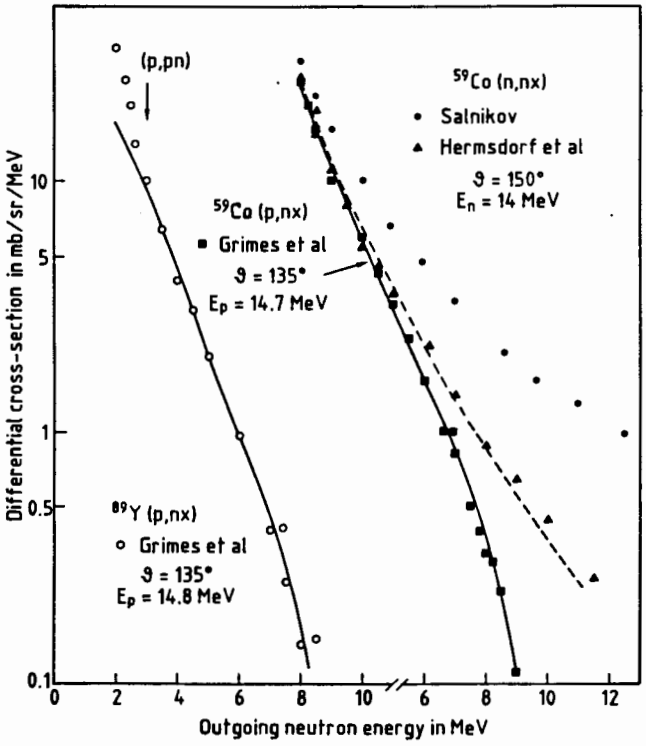

Fig.3. Differential cross-sections for the ^{89}Y(p,xn), ^{59}Co(p,xn) and ^{59}Co(n,xn) reactions compared with multistep compound calculations. In the case of ^{59}Co(n,xn) the difference between the data of Salnikov *et al* and that of Hermsdorf *et al* makes reliable comparison impossible. In the case of the ^{89}Y(p,xn) reaction, neutrons from the (p,pn) reaction contribute to the measured cross-section at outgoing proton energies below that indicated by the arrow; these were not included in the calculation.

Several improvements have recently been made to the FKK theory (Hodgson and Chadwick, 1988; Chadwick, Bonetti and Hodgson, 1988), in particular the inclusion of the distinction between neutrons and protons in the intra-nucleus cascade. The wavefunctions of the interacting nucleons that appear in the transition matrix elements are calculated as eigenfunctions of a harmonic oscillator potential for the bound nucleons and from an opti-

cal model potential for the free nucleons. Also included is the restriction of excitons to bound states, which modifies the Williams formula. Thus for multistep compound processes the particles above the Fermi sea are restricted to energies less than their binding energy in the nucleus, and holes are restricted to energies greater than the depth of the potential. Some calculations made with the improved theory are compared with experimental data in figs.3 and 4.

There is considerable uncertainty concerning the comparison between theory and experiment for the more energetic emitted particles. There are sometimes significant differences between different sets of experimental data, and as long as these persist it is impossible to make a

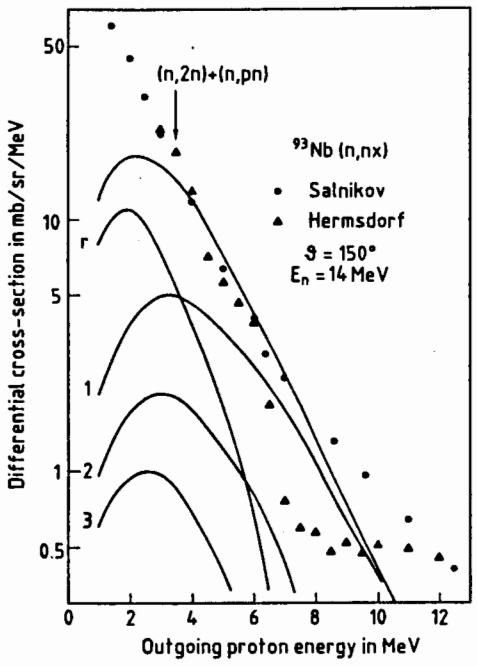

Fig. 4 Differential cross-section for the ^{93}Nb(n,nx) reaction compared with multistep compound calculations. The theory and experiment agree well for outgoing energies between 4 and 6 MeV but at higher energies the data are discrepant. Below 3.5 MeV the data includes contributions from the $(n,2n)$ and (n,pn) reactions, which are not included in the calculation.

reliable test of theories (see Fig.3). There is an appreciable contribution to the cross-section in this energy region from collective excitations, which may be treated more exactly by the coupled-channels formalism. Probably more important, in most cases, is the uncertainty due to the limitations of the expression used for the exciton level density. Detailed microscopic calculations by Reffo *et al*[49] taking into account the difference between neutron and proton cross-sections, and properly including the energies of particles and holes, show that the Williams formula is inadequate for the higher emission energies.

Much of the difficulty in interpreting the high energy end of the neutron spectra is associated with the rather poor energy resolution attainable. Bahm and Jahn[50] have pointed out the usefulness of analysing the corresponding proton emission spectra, which can be measured much more accurately. It is then possible to make a much more searching test of the various pre-equilibrium models.

The Multistep Direct Theory.

At higher energies it is increasingly likely that through out the reaction there is always at least one particle in the continuum. As before it is convenient to consider the reaction as taking place in a number of stages. The total emission cross-section is the sum of emissions in all stages, and may be written

$$\frac{d^2\sigma}{d\Omega d\epsilon} = \frac{d^2\sigma}{d\Omega d\epsilon_{\rm onestep}} + \frac{d^2\sigma}{d\Omega d\epsilon_{\rm multistep}}. \qquad (3.14)$$

We now introduce the cross-section for a transition from the $(N-1)$-th to the N-th stage and denote it by

$$W_{N,N-1} \equiv \frac{d^2W_{N,N-1}(\mathbf{k}_N,\mathbf{k}_{N-1})}{d\Omega d\epsilon}, \qquad (3.15)$$

where $\mathbf{k}_N$ is the particle momentum at the N-th stage.

If now we assume that retrograde processes are negligible, then the total multistep cross-section becomes

$$S_{\rm multistep} = \sum_N S_N = \sum_N \sum_{M=N-1}^{N+1} W_{MN}W_{N,N-1}\ldots W_{21}S_1 \qquad (3.16)$$

At each stage we must integrate over all angles and momenta, so that the full expression for the multistep cross-section is

$$\frac{d^2\sigma_{\rm if}}{dUd\Omega_{\rm multistep}} = \sum_N \sum_{M=N-1}^{N+1} \int \frac{d\mathbf{k}_1}{(2\pi)^3}\int \frac{d\mathbf{k}_2}{(2\pi)^3}\cdots\int \frac{d\mathbf{k}_N}{(2\pi)^3} \cdot\frac{d^2W_{MN}(\mathbf{k}_f,\mathbf{k}_N)}{dU_f d\Omega_f}\frac{d^2W_{N,N-1}(\mathbf{k}_N,\mathbf{k}_{N-1})}{dU_N d\Omega_N} \cdots\frac{d^2W_{2,1}(\mathbf{k}_2,\mathbf{k}_1)}{dU_2 d\Omega_2}\frac{d^2\sigma_{\rm if}}{dU_1 d\Omega_{\rm onestep}}. \qquad (3.17)$$

The transition matrix element

$$\frac{d^2W_{N,N-1}(\mathbf{k}_N,\mathbf{k}_{N-1})}{dU_N d\Omega_N} = 2\pi^2\rho(\mathbf{k}_N)\rho_N(U) < |v_{N,N-1}(\mathbf{k}_N,\mathbf{k}_{N-1})|^2 >, \qquad (3.18)$$

where $\rho(\mathbf{k}_N) = mk/(2\pi)^3\hbar^3$ is the density of particle states in the continuum, $\rho_N(U)$ the level density of the residual nucleus at excitation energy U and $v_{N,N-1}$ is the matrix element describing the transition from a state $N-1$ to a state N when the particle in the continuum changes its momentum from $\mathbf{k}_{N-1}$ to $\mathbf{k}_N$. This matrix element is given by the DWBA expression

$$v_{a,b}(\mathbf{k}_i,\mathbf{k}_f) = \int \chi_a^{(-)*} < \psi_f|V(r)|\psi_i > \chi_b^{(+)}d\mathbf{r}, \qquad (3.19)$$

where $V(r)$ is the effective interaction for the transition, $\chi_a^{(-)}$ and $\chi_b^{(+)}$ the incoming and outgoing distorted waves and ψ_i and ψ_f and initial and final nuclear states. To include all the transition strength, the spectroscopic factors are always taken to be unity.

In the expression (3.18) for the transition matrix element, the angular brackets indicate an appropriate averaging procedure. When the transition probability is averaged over many final states, the interference terms cancel and the orbital angular momenta contribute incoherently, so that the averaged value of the squared matrix element

becomes

$$< |v(\mathbf{k_i}, \mathbf{k_f})|^2 >= \sum_L < |v_L(\mathbf{k_i}, \mathbf{k_f})|^2 > S_L^N, \quad (3.20)$$

where S_L^N is the spin distribution function of the residual nucleus.

Similarly, the averaged single-step cross-section is given by

$$\frac{d^2\sigma_{\mathrm{if}}}{dU d\Omega_{\mathbf{singlestep}}} = \sum_L \rho_2^L(U) \left\langle \frac{d\sigma}{d\Omega_L} \right\rangle, \quad (3.21)$$

To evaluate this cross-section the angular distributions for each value of the transferred angular momentum are calculated by the distorted wave theory for particular ejectile energies and all possible particle-hole pairs formed by scattering between a particle in the continuum and a bound nucleon. The average of these cross-sections gives the last term in (3.21). A Yukawa potential with range 1 fm is usually taken for the residual interaction $V(r)$, and standard expressions are used for the state density and its spin distrtibution. The multistep cross-section is calculated in essentially the same way. Many multistep direct calculations have now been made in this way, and the results are in satisfactory overall agreement with the experimental date (Avaldi *et al*[44]; Bonetti *et al*[47]; Hollet *et al*[51]; Mordhost *et al*[52]; Marcinkowski[53]).

The Theory of Tamura

The cross-section of a nuclear reaction at high energies is the energy average of the sum of the cross-sections for exciting many complicated eigenstates, and statistical arguments can be used to justify approximating this by a sum of cross-sections to a much smaller number of simpler model states. For one-step transitions, Tamura and his colleagues use an expression of the form

$$\frac{d^2\sigma^{(1)}(E_b)}{dE_b d\Omega} = \sum_B C_B(Ex) \frac{d\sigma_B^{(1)}(E_B)}{d\Omega_b} \quad (3.22)$$

where $Ex = E_a - Q^B - E_b$, E_a and E_b being the incident and exit channel energies and Q^B the Q-value for transitions from the ground state of the nucleus A to the ground state of the nucleus B. For two-step transitions

$$\frac{d^2\sigma^{(2)}(E_b)}{dE_b d\Omega_b} = \sum_{BC} \int_{E_b-(Q^B-Q^C)}^{E_c-Q_c} C_B(Ex')C_C(Ex) \left\{ \frac{d\sigma_{BC}^{(2)}(E_b, E_c)}{d\Omega_b} \right\} dE_c \quad (3.23)$$

where $E_x' = E_c + Q^B - Q^C - E_b$ and $d\sigma_B^{(1)}/d\Omega_b$ and $d\sigma_{BC}^{(2)}/d\Omega_b$ are the first and second order DWBA cross-sections. The statistical assumption justifies neglecting the interference terms between amplitudes to different states B and C as well as between the one-step and two-step amplitudes. The coefficient $C_B(E_x)$ is the probability per unit energy that there is a state B at excitation E_x.

These expressions may be further simplified by removing the dependence on B and C of the elementary cross-sections. This reduces the above expressions to

$$\frac{d^2\sigma^{(1)}(E_b, Q_\ell)}{dE_b d\Omega_b} = \sum_J \rho_J(E_x) \frac{d\sigma_J^{(1)}(E_b, Q_b)}{d\Omega_b} \quad (3.24)$$

and

$$\frac{d^2\sigma^{(2)}(E_b, Q_\ell)}{dE_b d\Omega_b} = \sum_{J_1 J_2} \int dE_c \rho_{J_1}(E_x) \rho_{J_2}(E_x') \sum_J \frac{d\sigma_{J_1 J_2; J}^{(2)}(E_\ell, E_c, Q_\ell)}{d\Omega_\ell} \quad (3.25)$$

where $\rho_J(E_x) = \sum_B C_B(E_x)(d_J^{BA})^2$ is the spectroscopic density, and d_J^{BA} is the spectroscopic amplitude and $J \equiv \{\ell_{sj}\}$ is the set of orbital, spin and total transferred angular momenta.

The early calculations assumed angular momentum independent form factors and a simple model for $\rho_J(E_x)$.

This theory has been used by Tamura *et al*[43] to analyse several (p, p') and (p, α) cross-sections at 62 MeV and (n, n') and (p, n) data at lower energy, with generally satisfactory results, apart from some difficulties with the absolute magnitude of the cross-sections that may be attributed to the assumption that the form factors are independent of the angular momentum[54]. In several cases, such as for the (p, α) reaction at 34.6 and 44.3 MeV and the (n, p) reaction at 26 MeV, the cross-section can be adequately fitted by combining the single-step direct cross-section with the compound nucleus contribution[55].

General Comments

The quantum-mechanical theories of pre-equilibrium reactions enable both the multistep compound and multistep direct contributions to be calculated. For medium weight nuclei the multistep compound process dominates at around 15 MeV and as the energy increases the multistep direct becomes increasingly important until by about 25 MeV it is the dominant process. There are however some forward-peaked angular distributions for reactions on heavier nuclei around 11–14 MeV that indicate the presence of substantial direct components even at such comparatively low energies.

Sufficient analyses have now been made at 14 MeV to enable the cross-sections of multistep compound reactions on medium weight nuclei to be calculated with some confidence, the main uncertainty being in the absolute magnitude due to uncertainties in the level density parameters. However for the dominant (n, n') reaction the magnitude of the cross-section is limited by the known total cross-section, so this uncertainty is not so important.

At higher energies, where the direct processes dominate, the theories are able to give the angular distributions of the cross-sections quite well, but there are still considerable difficulties in predicting their absolute magnitudes.

4. Computer Programs

Many computer programs have been written to carry out numerical calculations with the theories described in the previous two sections, and they have been applied extensively to analyse experimental data.

It is essential that any computer program be checked most carefully to ensure that it accurately calculates what it is supposed to calculate. Many programs are now being tested under the auspices of the Nuclear Data Bank in Paris, and the results are in course of publication. It is only after the correctness of a program has been verified that it is useful to compare its predictions with experimental data.

A very thorough intercomparison of computer pro-

grams for pre-equilibrium calculations was made by Gruppelaar and Nagel[56] and more recently by Vonach[57]. The programs examined are listed in Table 4.1. The programs are divided into three classes: A: Hauser-Feshbach with precompound and unified models; B: Excitation Model; and C: Geometry-dependent Hybrid Model. Those in the first class A incorporate angular momentum conservation and can give cross-sections to discrete final states but are time-consuming to run. Most of them give the energy- and angle-integrated cross-section, the angle-integrated particle spectra, multiparticle emission and gamma-ray cascades. Those in class B do not include explicit angular momentum conservation and are simple and fast, and they often treat the pre-equilibrium aspects in a more sophisticated way than Class A programs. Those in Class C have energy-dependent transition rates that refer to the individual particle, rather than the nucleus as a whole, and they also include surface effects.

TABLE 4.1

A: HF + Precompound	B: Exciton Model	C: Geometry-dependent Hybrid Model
STAPRE	PREM (TOH)	ALICE (LLL)
GNASH	PRECO-D2 (TNL)	SECDIST (KfK)
HAUSER V	PREANGI (TRM)	EMPIRE
PERINNI	PRANG (ECN)	
TNG (DRL)	PEQGM (SLO)	
EMPIRE	AMPRE (TUD)	

In the comparison of Gruppelaar and Nagel the cross-sections of the (n,n'), $(n,2n)$, (n,p) and (n,α) reactions at 10, 14.6, 20 and 25.7 MeV calculated with each of these programs were tabulated. With a few exceptions, the cross-sections of the dominant (n,n') and $(n,2n)$ reactions were consistent to about $\pm 5\%$, whereas those of the much smaller (n,p) and (n,α) reactions showed much larger differences, that mainly reflect important differences between the various models of the reaction. These are discussed in detail by Gruppelaar and Nagel, and a summary of the main conclusions may be found in Gruppelaar, Nagel and Hodgson[58].

The choice of program depends on the type of experimental data to be analysed. If these are angle-integrated total emission spectra, the exciton and geometry-dependent hybrid models are the most suitable. If angular distributions are also available, it is possible to distinguish between the multistep compound and multistep direct contributions to the cross-section, and the programs GNASH, PRECO-D2, TNG, PRANG, ALICE (LLL) and AMPARE may be used. In their review Gruppelaar and Nagel compare the angular distributions calculated with all these programs. It is generally found, however, that these programs have difficulty in fitting the angular distributions in the backward direction, due to the semi-classical nature of the theories they use. This can be corrected by the introduction of empirical factors.

The programs for the quantum-mechanical calculations are not yet generally available.

In addition to the intercomparison carried out by Gruppelaar and Nagel, that was concerned principally with comparing different theories, there have been other comparisons concerned with establishing the comparative accuracy of different programs using the same formalism. These are listed in Table 4.2[59].

5. Conclusions

In the last few years there has been an extensive development of theories of pre-equilibrium reactions, and many computer programs have been written to enable the cross-sections to be calculated.

The semi-classical models are now reaching the stage that they successfully describe and predict the double-differential cross-sections of continuum emission for most technological applications. However, existing experimental information, *e.g.* the extensive set of 14.5 MeV data, has been used to tune parameters and to add or neglect certain effects. Recently, the relations between EM and GDH have been clarified (see Akkermans[36]; Bisplinghoff[17]) The success of the GDH model in describing the high-energy tail of the spectrum could be a reason to adopt similar effects also in the exciton model (Kalbach[31]). An important field of further study is the introduction of angular-momentum conservation in the model and the improvement of particle-hole level density expressions. Angular distributions are reasonably well described by some of the recent models.

TABLE 4.2
Computer Code Intercomparisons

Nuclear Theory	Author
Statistical Model	Prince *et al*, 1983
Coupled-Channels	Sartori, 1984
Optical Model	Hodgson and Sartori, 1986
Pre-Equilibrium	Gruppelaar *et al*, 1986
Weisskopf-Ewing and Hauser-Feshbach	Hodgson and Sartori (in progress)

The QM theories have now been developed to the stage when it is possible to calculate unknown cross-sections with some confidence. They are being extensively tested and extended to a wider-range of reactions.

The quantum-mechanical theories now make possible an overall survey of the magnitudes of the MSC and MSD processes as a function of energy for a range of nuclei, together with the relative importance of one-step and multistep processes. This information is helpful in deciding which theory to apply to a particular data set. It is likely that in many applications below 20 MeV one could use MSC and only one-step direct continuum theory (Tamura *et al*[43]). For $(n,2n)$ and (n,np) reactions probably only MSC is required (Herman *et al*[48]).

Relations between semi-classical and QM models.

The quantum-mechanical theories grew out of the semi-classical theories and remain strongly influenced by them, and there is a corresponding influence back onto the semi-classical theories. Thus the distinction between the MSC and MSD first made by FKK led to the successful phenomenological parametrization of the angular distributions of these two processes by Kalbach and Mann[28]. At present one could make a further step by checking and subsequently improving the MSC component angular distributions after studying the results from MSC calculations. This applies to all three semi-classical methods mentioned before. It sometimes happens that the quantum-mechanical calculations suggest simplifications in the semi-classical theories by showing that some quantity is practically independent of a particular variable. For example, the work of Herman *et al*[48] showed that the

escape and damping widths are practically independent of J, and this enables the calculation of the τ^{J_π} and W^{J_π} to be greatly simplified without appreciable loss of accuracy (Gruppelaar and Akkermans[27]). Furthermore, the weak n-dependence of the damping widths could be used to check the various ways in which $\lambda+$ are evaluated in the EM and GDH models.

Applicability and predictive power.

The theories differ appreciably in their flexibility, in several different respects. The semi-classical theories have been applied to a much wider range of reactions than the quantum-mechanical theories, in particular to those initiated by complex particles and those leading to the emission of many particles. By contrast, the quantum-mechanical theories have so far been confined to nucleon interactions with not more than two emergent particles. In the next few years the quantum-mechanical theories will certainly be applied to a wider range of reactions, but at present the semi-classical theories are the only ones that can be used for a wide range of reactions.

The semi-classicall theories are also more flexible in that they have more model parameters than the quantum-mechanical theories. Here one must distinguish between parameters that are *special* to the particular theory and those that are fixed by some *external* constraint. There is a further distinction that is important for the predictive power of these theories: reliable global optical potentials are now available for nucleons os that the cross-sections can be calculated from them for any nucleons with good accuracy. It is, of course, possible to improve the accuracy in particular cases by further parameter adjustment, but in general the increased accuracy does not outweigh the lower predictive power. The particle-hole level density parameters, on the other hand, cannot be represented with sufficient accuracy by global formulae and only the total level density could be fitted to the experimental data for each nucleus. Therefore, there is a strong need to obtain reliable expressions for these particle-hole level densities, in particular for the llowest stages. These considerations apply both to the semi-classical and to the quantum-mechanical theories.

If all that is required is a fit to a particular data set, this can be achieved by both the semi-classical and the quantum-mechanical theories for the energy distributions of the emerging particles. The semi-classical calculation may require some adjustment of a *special* parameter, and both types are subject to the above remarks about *external* parameters, particularly those relating to particle-hole level densities. In practice the range of applicability of the semi-classical models is often well known and it is not necessary to adjust *special* model parameters in each computation.

With respect to *angular distributions* the quantum-mechanical effects may be more important. The most recent descriptions in EM and GDH are based upon the scattering in infinite nuclear matter with quasi-classical descriptions of refraction and/or finite-size effects. Conceptually the QM theories are, of course, superior. In particular, there are difficulties in the description of back-angle cross-sections with the semi-classical theories, that do not exist in QM theories. This was illustrated recently by Holler *et al*[51] in comparison with semi-classical and quantum-mechanical pre-equilibrium calculations for ^{65}Cu(p,xn) at 26.7 MeV. The GDH model of Blann and Vonach[33] gives a good overall fit to the energy distribution of the emitted neutrons, but is unable to fit the angular distribution in the very forward and backward directions. The back angle discrepancy persists when refraction and finite-size effects are included in the calculations. Quantum-mechanical calculations with the FKK theory are, however, able to fit the data over the whole angular range, showing that they are able to evaluate interference effects that are beyond the scope of the semi-classical theories.

The theories of pre-equilibrium reactions are now in a stage of complex and fruitful development. Within their more limited domain, the quantum-mechanical theories give a truer account of the underlying physics and enable the cross-sections and angular distributions to be calculated with some accuracy and confidence. Extension to other reactions will certainly be made, but at the expense of still greater computational complexity.

The semi-classical theories are conceptually simpler, more flexible and the corresponding computer programs are generally much faster. One may imagine that EM and QM could be used in a complementary way: EM for fast global computations supplemented by QM when greater detail and accuracy is required. Further improvements will certainly be made as these theories are critically compared with each other, and as simplifying assumptions validated by the quantum-mechanical theories are incorporated into their structures.

At the same time as the formalisms are developed and improved, the accurate of prediction will be improved as extensive analyses of new and more accurate data yield better values of the parameters of the theories. This in turn should stimulate theoretical work on more fundamental lways of understanding and determining these parameters, with the consequent development of more accurate and reliable global prescriptions.

I am grateful to Dr H. Gruppelaar, Dr P. Nagel and Mr M.B. Chadwick for kindly permitting me to include in this review some sections from our joint papers[46,58].

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