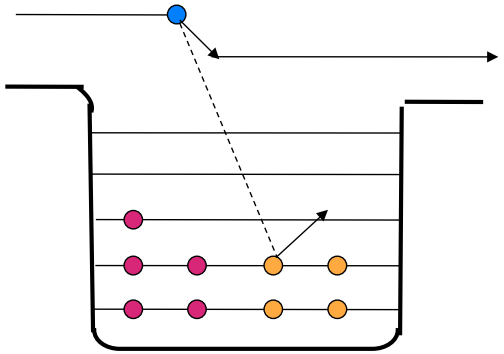
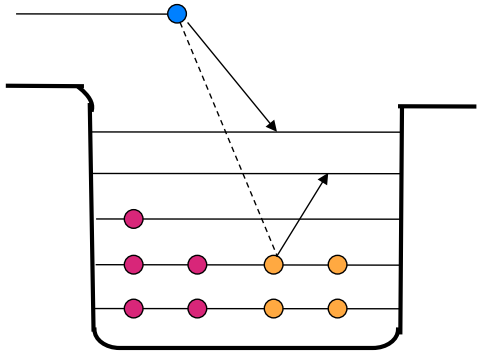
Semiclassical models of



pre-equilibrium emission



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Pre-equilibrium emission

At low incident energy, nuclear reactions occur on two distinct time scales. Direct reactions, in which the incident particle remains in the continuum, occur quickly. Compound nucleus reactions, in which the projectile is trapped in a quasi-bound state, occur much more slowly.

The corresponding differential cross sections are consistent with their time scales: direct reactions tend to be forward peaked while compound nucleus ones are symmetric about 90°.

Preequilibrium processes corresponding to intermediate time scales arise and become ever more important as the incident energy increases.

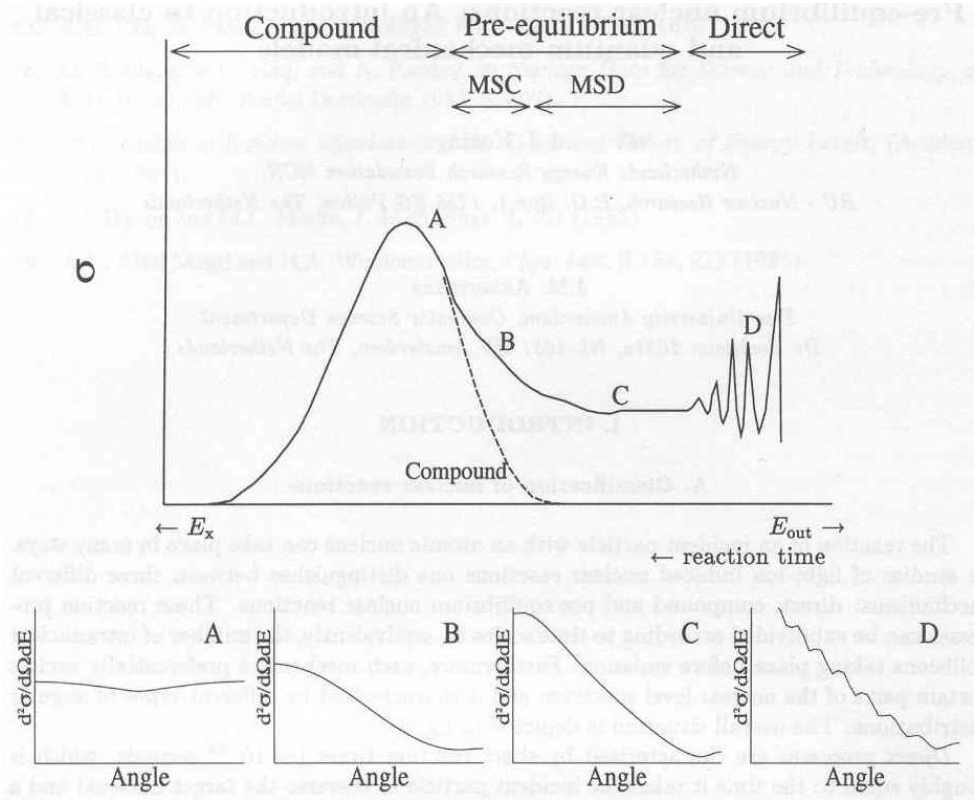
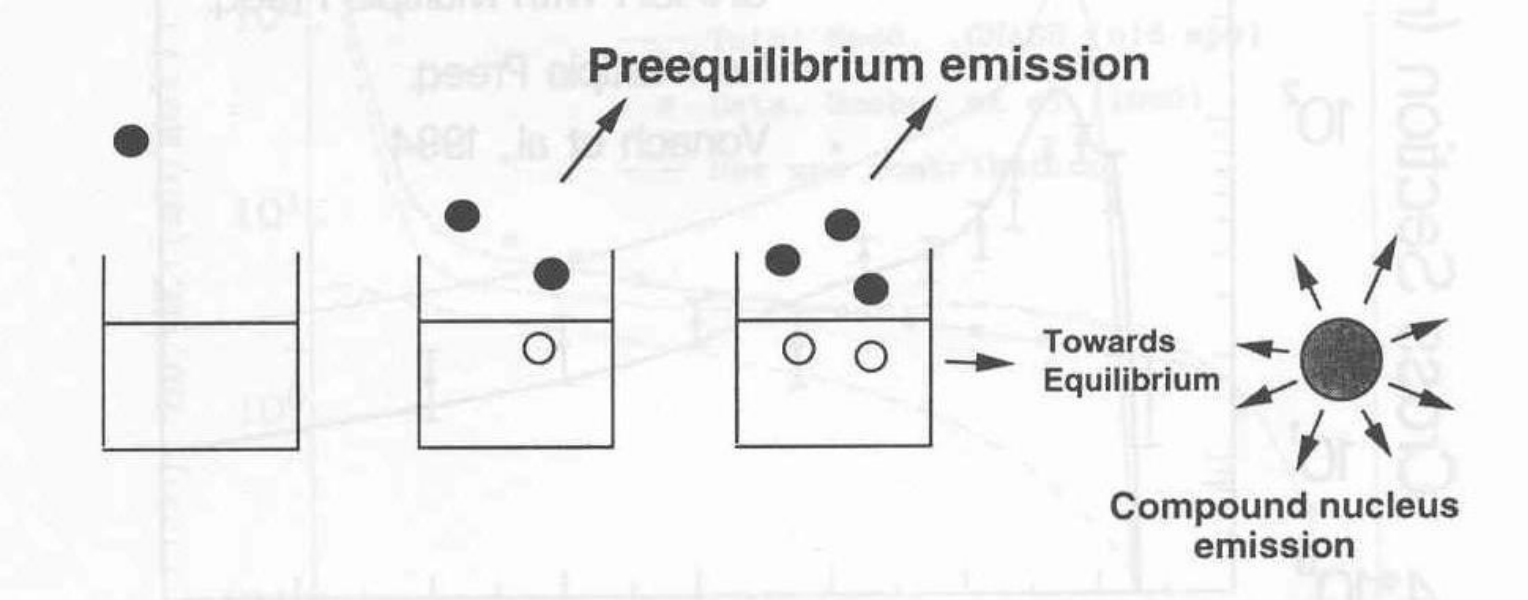


Figure from A. J. Koning,,J. M. Akkermans, ICTP Workshop, 1998.

Preequilibrium emission



Compound nucleus models assume that the nucleus reaches an equilibrium (all states are equally probable) before emission occurs.

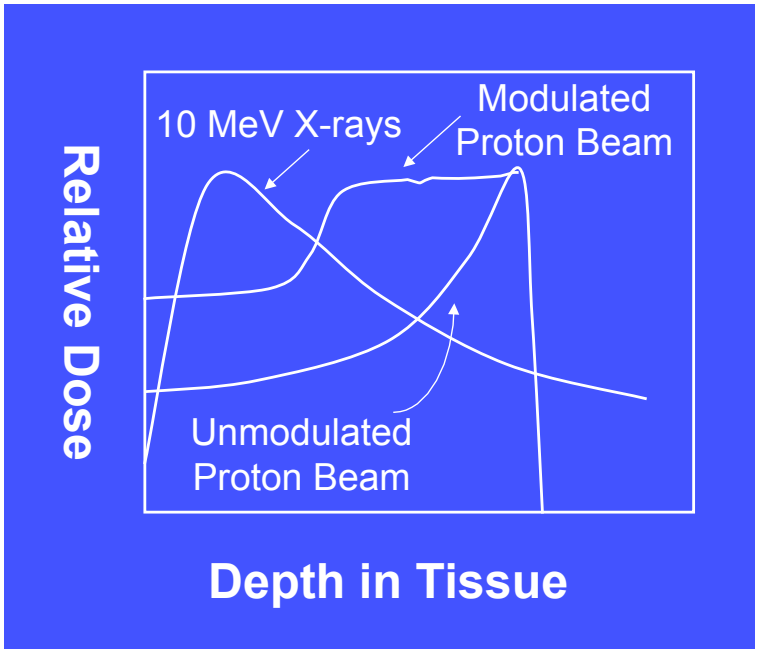
Physically, the equilibration process proceeds through a series of nucleon-nucleon reactions. As the incident energy increases, it becomes more and more likely that one of the nucleons still retains a large fraction of the incident energy after the first one or two collisions, which favors its emission from a preequilibrium configuration.

Nucleon-induced pre-equilibrium reactions

- nucleons are emitted before the energy is equally distributed among all active degrees of freedom;
- pre-equilibrium nucleons tend to be more energetic;
- angular distributions are forward peaked.

Nucleon-induced pre-equilibrium reactions are most important above about 10 MeV -

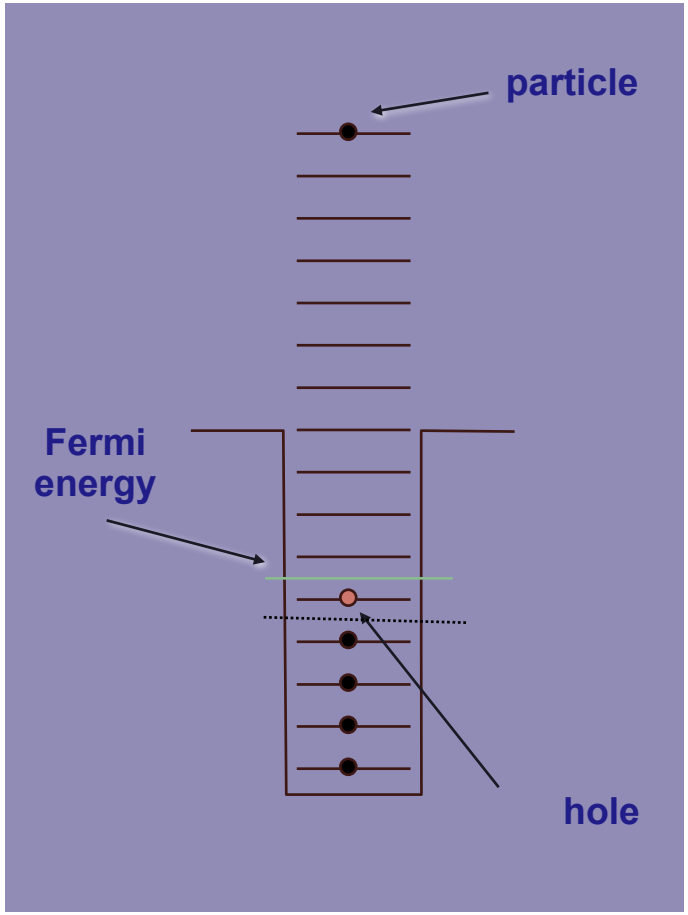
- fast reactors,
- accelerator-driven systems (ADS),
- proton radiation therapy,
- space applications (cosmic rays).



Taken from a presentation by R.W. Schulte

The exciton model

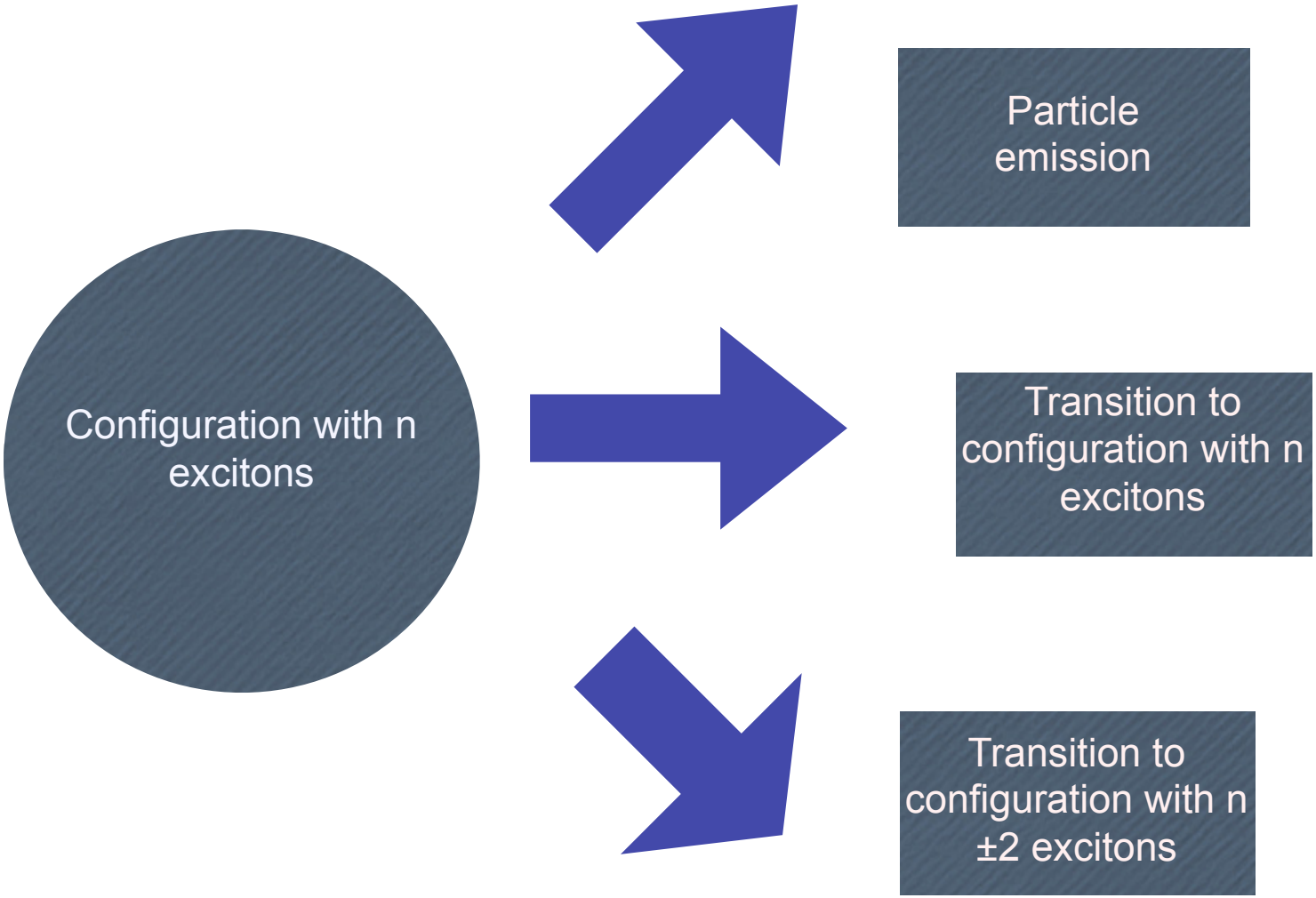
- Nucleons occupy single-particle states ;
- The Fermi energy is between the last occupied and first unoccupied level of the target ground state;
- Particles are nucleons above the Fermi energy and holes are unoccupied states below it. Both are called excitons;
- The hole at the Fermi energy corresponding to the incident particle is not taken into account;



We call the set of configurations with the same number of excitons an **exciton class**.

J.J. Griffin, Phys. Lett. **17** (1966) 478.

A reaction proceeds through energy-conserving two-nucleon collisions and eventual emission.



The first few stages of a pre-equilibrium reaction

The rate of particle emission is a product of two factors:

1) the transmission frequency -

$$\frac{\sigma(\varepsilon)\,v}{V} \propto \frac{1}{V}\int \hat{r}\cdot\vec{v}\,\delta(r-R)\,d^3r$$

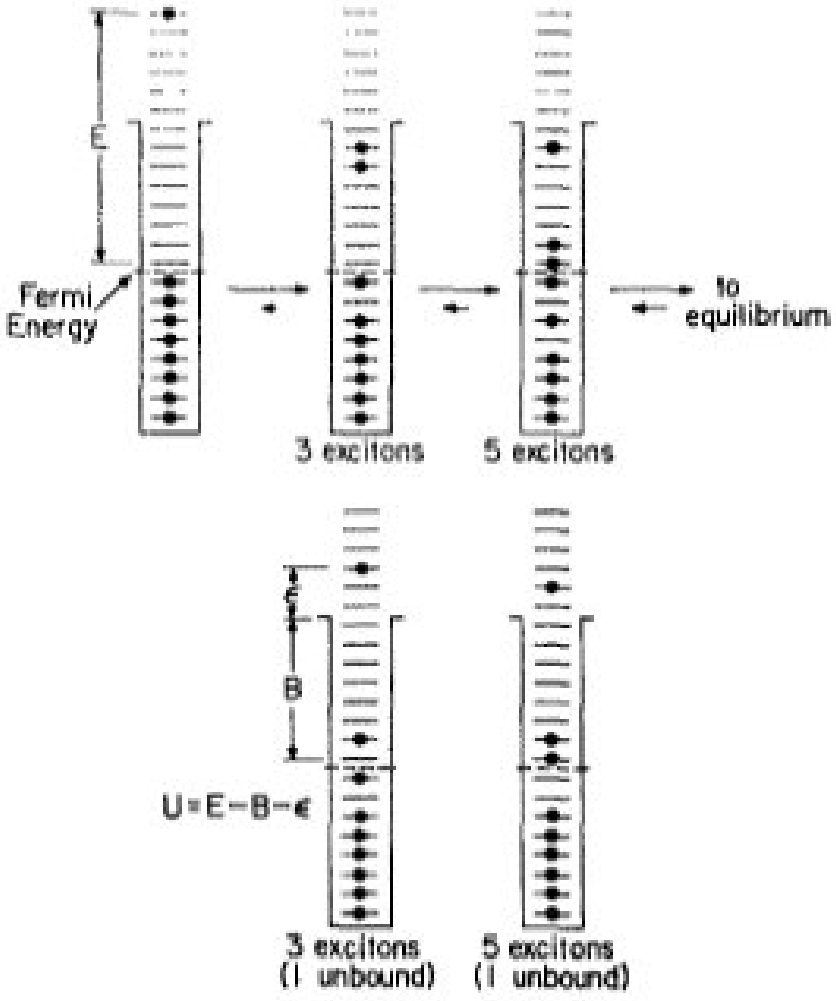
2) the ratio of final to initial states -

$$\frac{\omega(n-1,U)}{\omega(n,E)}\underbrace{(2s+1)\frac{V\,4\pi p^2 dp}{(2\pi\hbar)^3}}$$

free particle phase space

where

$$U = E - B - \varepsilon$$



From C.K.Cline and M. Blann, Nucl. Phys.**A172**(1971)225.

The pre-equilibrium emission spectrum

Simplifying, we write the differential emission rate from the n-exciton class as

$$\frac{d\lambda_e}{d\varepsilon}(n,\varepsilon)d\varepsilon = (2s+1)\frac{\mu\varepsilon\sigma(\varepsilon)}{\pi^2\hbar^3}d\varepsilon\frac{\omega(n-1,U)}{\omega(n,E)}$$

This is just the Weisskopf emission rate, but with exciton densities of states rather than equilibrium ones.

If we now multiply by the average time spent in the n-exciton configuration and sum over all possible exciton numbers, n=3, 5, 7, …, we obtain the spectrum of emitted particles,

$$N(\varepsilon)d\varepsilon \propto (2s+1)\frac{\mu\varepsilon\sigma(\varepsilon)}{\pi^2\hbar^3}d\varepsilon\sum_n\frac{\omega(n-1,U)}{\omega(n,E)}\tau_n$$

However, to determine the average time spent in an exciton class, we must know how to calculate the rate of transitions between classes. To determine the emission rates, we also must know the exciton densities of states. We will begin with these.

Exciton state densities - I

The simplest estimate of the density of states of an n-exciton class assumes contant single-particle and single-hole densities and the constraint of energy conservation. We must also take into account that holes and particles are each indistinguishable.

For a two-particle – one-hole density, we have,

$$\omega(p=2,h=1,E)=\frac{g_p^2 g_h}{2!1!}\int d\varepsilon_{p1}d\varepsilon_{p2}d\varepsilon_{h1}\delta(E-\varepsilon_{p1}-\varepsilon_{p2}-\varepsilon_{h1})=\frac{g_p^2 g_h E^2}{2!1!2!}$$

which we can generalize immediately to

$$\omega(p,h,E)=\frac{g_p^p g_h^h}{p!h!}\int\prod_{j=1}^{p}d\varepsilon_{pj}\prod_{k=1}^{h}d\varepsilon_{hk}\,\delta\left(E-\sum_{j=1}^{p}\varepsilon_{pj}-\sum_{k=1}^{h}\varepsilon_{hk}\right)$$

$$=\frac{g_p^p g_h^h E^{n-1}}{p!h!(n-1)!}$$

Usually $g_p=g_h=g$

T. Ericson, Adv. Phys. **9** (1960) 425.

Exciton state densities - II

Although the densities on the previous slide take into account the indistinguishability of the particles and of the holes, they do not take into account the Pauli exclusion principle.

Williams obtained the corrected densities by considering an equally spaced set of single-particle levels. This is

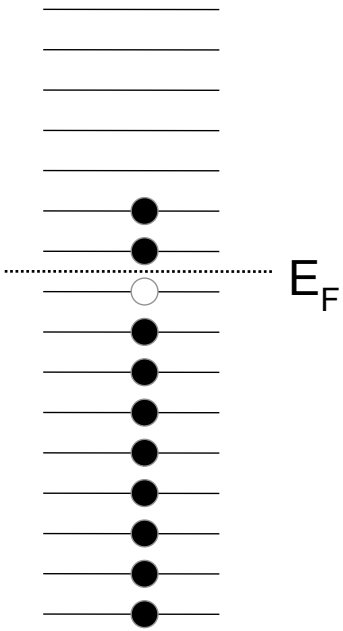
$$\omega(p,h,E) = \frac{g^n \left(E - A_{p,h}\right)^{n-1}}{p!h!(n-1)!}$$

where the Pauli blocking correction is

$$A_{p,h} = \frac{1}{4g}[p(p-1) + h(h-1)]$$

when the Fermi energy E_F is placed symmetrically between the last occupied and first unoccupied levels.

Here, we show the lowest 2p-1h state at E=5/(2g).



F.C. Williams Jr., Nucl. Phys. **A166** (1971) 231.

Exciton state densities - III

Still another effect that must be taken into account at higher energies is the that fact that the single-particle hole states are limited to the depth of the potential.

Beták and Dobes obtained the corrected density as

$$\omega(p,h,E) = \frac{g^n}{p!h!(n-1)!}\sum_{j=0}^{h}(-1)^j\binom{h}{j}\left(E - jV - A_{p,h,j}\right)^{n-1} \times\theta\left(E - jV - A_{p,h,j}\right)$$

where the Pauli correction terms are different for each value of j.

Kalbach approximated this as

$$\omega(p,h,E) = \frac{g^n\left(E - A_{p,h}\right)^{n-1}}{p!h!(n-1)!}f(p,h,E)$$

with

$$f(p,h,E) = \sum_{j=0}^{h}(-1)^j\binom{h}{j}\left(\frac{E-jV}{E}\right)^{n-1}\theta(E-jV)$$

E. Beták and J. Dobes, Z. Phys. **A279** (1976) 319.
C. Kalbach, BNL Report BNL-NSC-51694 (1983) 113.

The master equation

The exciton model was cast in the form of an energy-conserving, time-dependent master equation by Cline and Blann.
The equation governing the time development of the fraction of the probability P(n) in the n-exciton class takes into account transitions that increase or decrease the number of excitons by two, transition that don't change the number of excitons and, finally, loss due to emission.

$$\frac{dP(n)}{dt} = \lambda_-(n+2)\,P(n+2) + \lambda_0(n)\,P(n) + \lambda_+(n-2)\,P(n-2) - \tilde{\lambda}(n)\,P(n)$$

where the total width is

$$\tilde{\lambda}(n) = \lambda_-(n) + \lambda_0(n) + \lambda_+(n) + \lambda_e(n),$$

However, the transitions that do not change the exciton number cancel, so that we can write

$$\frac{dP(n)}{dt} = \lambda_-(n+2)\,P(n+2) + \lambda_+(n-2)\,P(n-2) - \lambda(n)\,P(n)$$

with $\lambda(n) = \lambda_-(n) + \lambda_+(n) + \lambda_e(n)$ and $n = p + h$

C.K. Cline and M. Blann, Nucl. Phys. **A172** (1972) 225.

Transition rates - I

We assume that the states in each exciton class are in equilibrium and that transitions are induced by energy-conserving two-body interactions.

We then have for the transition rate that increases the exciton number by two,

$$\lambda_+(n) = \frac{2\pi}{\hbar}|M|^2 \int_0^E d\varepsilon \left(\omega(2,1,\varepsilon)\frac{\omega(1,0,\varepsilon)\omega(p-1,h,E-\varepsilon)}{\omega(n,E)} + \omega(1,2,\varepsilon)\frac{\omega(0,1,\varepsilon)\omega(p,h-1,E-\varepsilon)}{\omega(n,E)} \right)$$

We calculate the transition rate that decreases the exciton number by two as

$$\lambda_-(n+2) = \frac{2\pi}{\hbar}|M|^2 \int_0^E d\varepsilon \left(\omega(1,0,\varepsilon)\frac{\omega(2,1,\varepsilon)\omega(p-1,h,E-\varepsilon)}{\omega(n+2,E)} + \omega(0,1,\varepsilon)\frac{\omega(1,2,\varepsilon)\omega(p,h-1,E-\varepsilon)}{\omega(n+2,E)} \right)$$

and note that

$$\omega(n,E)\,\lambda_+(n) = \omega(n+2,E)\,\lambda_-(n+2)$$

Transition rates - II

We can thus write

$$\begin{aligned}\omega(n,E)\,\lambda_+(n) &= \omega(n+2,E)\,\lambda_-(n+2)\\ &= \frac{2\pi}{\hbar}|M|^2\int_0^E d\varepsilon\,(\omega(2,1,\varepsilon)\omega(1,0,\varepsilon)\omega(p-1,h,E-\varepsilon)\\ &\qquad +\omega(1,2,\varepsilon)\omega(0,1,\varepsilon)\omega(p,h-1,E-\varepsilon))\end{aligned}$$

Although it does not enter the master equation, we can write the transition rate that leaves the exciton number the same in a similar manner,

$$\begin{aligned}\omega(n,E)\,\lambda_0(n) = \frac{2\pi}{\hbar}|M|^2\int_0^E d\varepsilon\,&(\omega(2,0,\varepsilon)\omega(2,0,\varepsilon)\omega(p-2,h,E-\varepsilon)\\ &+\omega(1,1,\varepsilon)\omega(1,1,\varepsilon)\omega(p-1,h-1,E-\varepsilon)\\ &+\omega(0,2,\varepsilon)\omega(0,2,\varepsilon)\omega(p,h-2,E-\varepsilon))\end{aligned}$$

The emission width is the integral of the expression we obtained earlier

$$\lambda_e(n) = (2s+1)\int \frac{\mu\varepsilon\sigma(\varepsilon)}{\pi^2\hbar^3}\,\frac{\omega(n-1,E-B-\varepsilon)}{\omega(n,E)}\,d\varepsilon$$

The matrix element - $|M|^2$

The calculation of the transition rates assumed an average matrix element that could be taken out of the integral.

An early parametrization obtained by comparison with data by Kalbach-Cline is

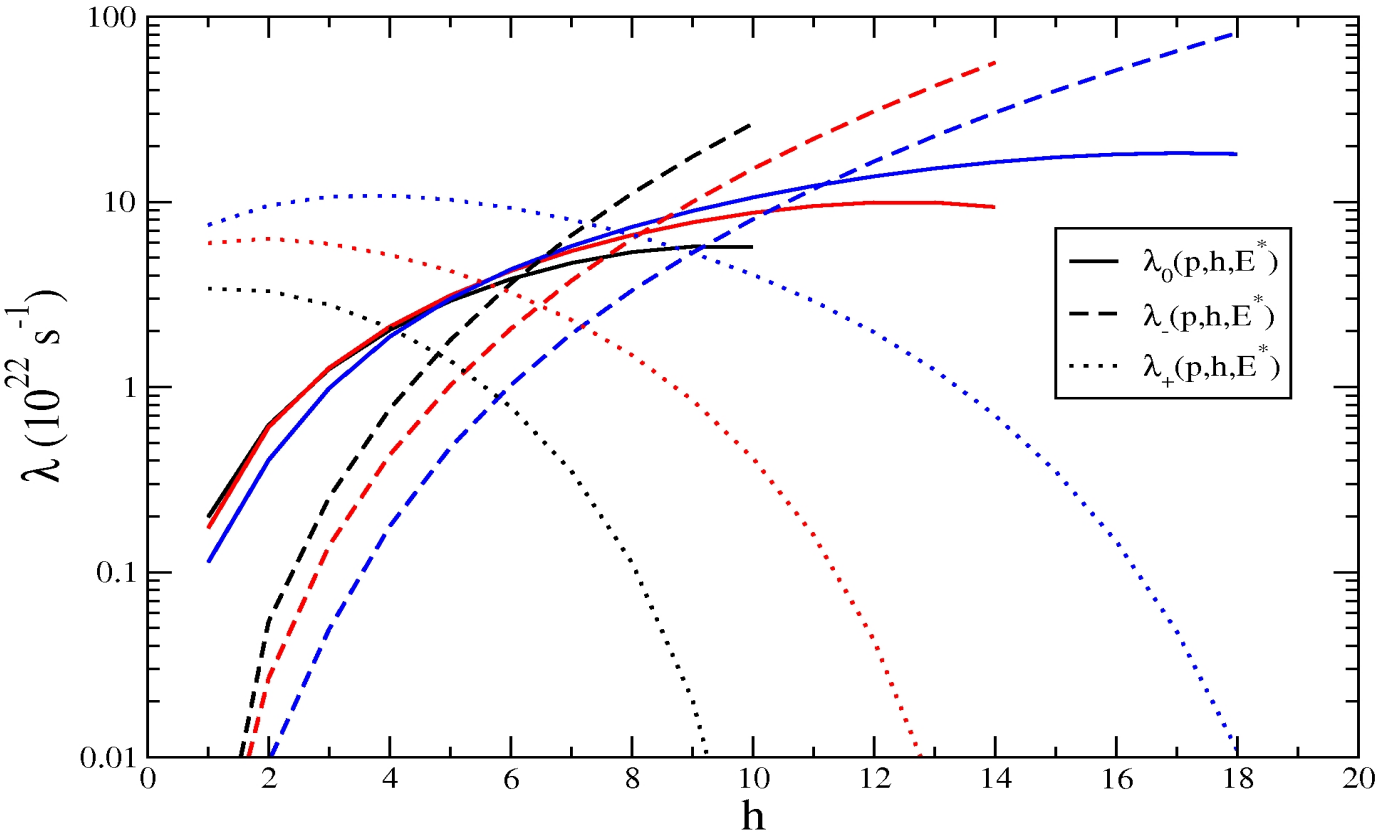
$$|M|^2 = \frac{f_M}{A^3 E} \qquad \text{with} \qquad f_M = 230\ \text{MeV}^3$$

The dependence on the nuclear mass A is the dependence expected of two-body shell model matrix elements. The energy dependence is phenomenological. More elaborate parametrizations of the matrix element can be found in the literature.

The matrix elements coupling states are obviously not so simple as to be represented by a single number. We will come back to this subject again.

C. Kalbach-Cline, Nucl. Phys. A210 (1973) 590.

Transition rates - III



Transition rates for nucleon + ^{40}Ca

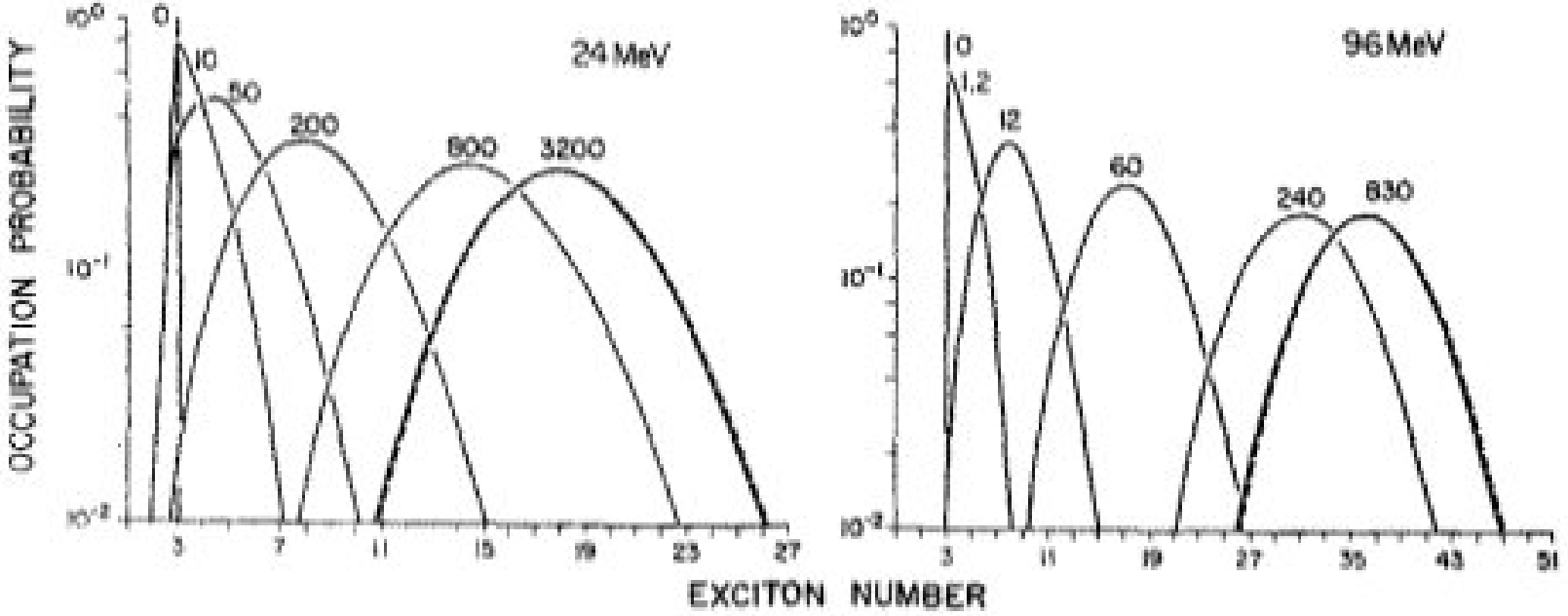
- Incident energies of 25, 50 and 100 MeV.

Solutions of the master equation

Two solutions to the master equation are shown for a nucleus of mass number A ≈ 90 and excitation energies of 24 Mev and 96 MeV.

In both cases, the system is initially in the 2p-1h, 3 exciton class. The time step was chosen arbitrarily.

The “equilibrium” solution is given by the dashed line.



From C.K.Cline and M. Blann, Nucl. Phys.**A172**(1971)225.

Equilibrium solution

Let us assume for the moment that the particle emission rate is zero for all exciton classes. The master equation can then be written as

$$\frac{dP(n)}{dt} = \lambda_-(n+2)\,P(n+2) + \lambda_+(n-2)\,P(n-2) - (\lambda_+(n) + \lambda_-(n))\,P(n)$$

Recalling the identity,

$$\omega(n,E)\,\lambda_+(n) \;=\; \omega(n+2,E)\,\lambda_-(n+2)$$

we see that when

$$P(n) \propto \omega(n,E)$$

we have equilibrium,

$$\frac{dP(n)}{dt} = 0$$

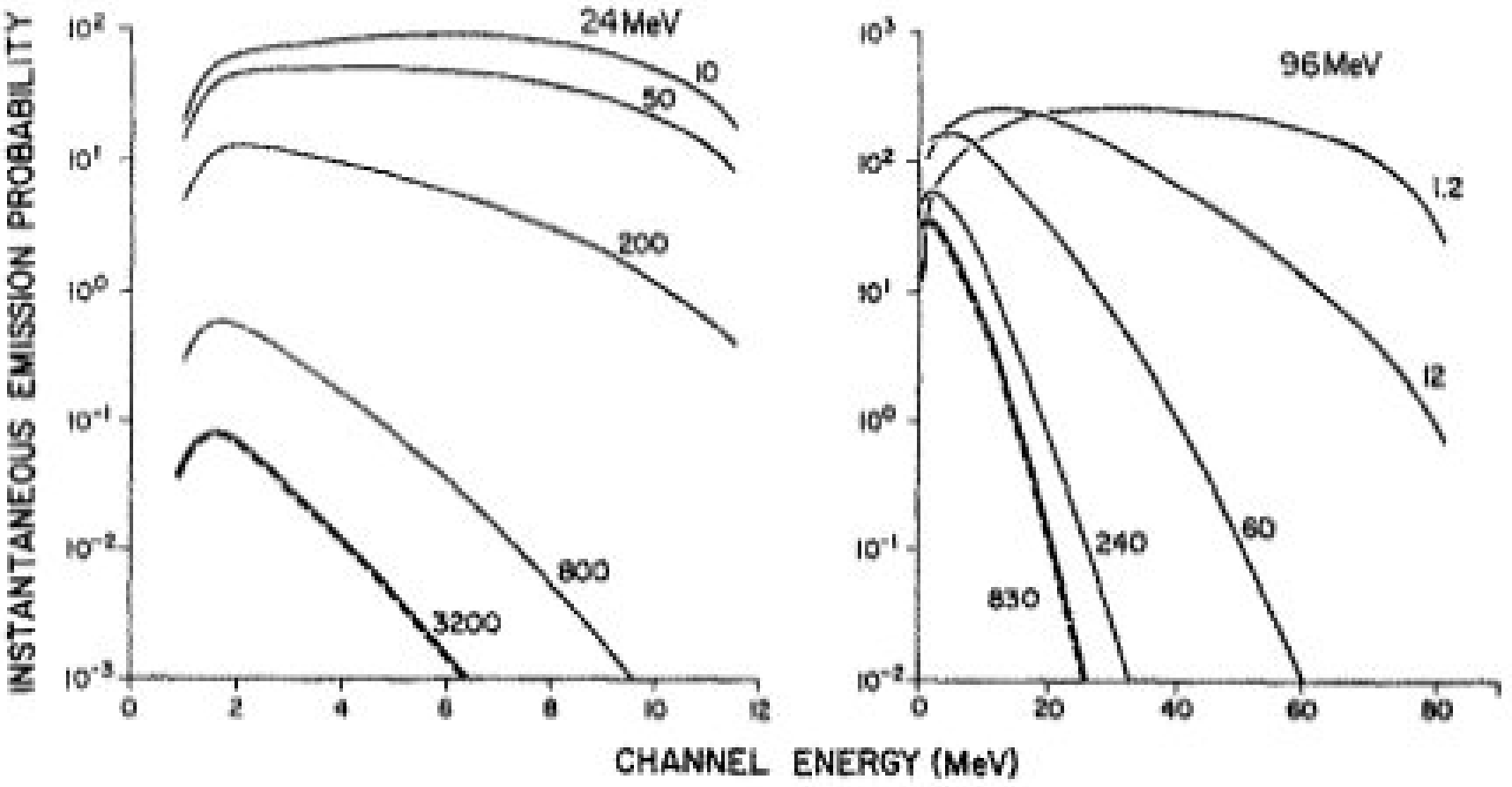
When the particle emission rates are small compared to the transition rates, the system will evolve to the normalized equilibrium solution before decaying,

$$P(n,t) \to \frac{\omega(n,E)}{\omega_{tot}(E)} \qquad \text{where} \qquad \omega_{tot}(E) = \sum_{n=3,5,\ldots} \omega(n,E)$$

Instantaneous emission rates

The instantaneous emission spectrum is given by

$$\frac{d\lambda_e}{d\varepsilon}(\varepsilon) = \sum_{n=3,5,\ldots} \frac{d\lambda_e}{d\varepsilon}(n,\varepsilon)P(n,t)$$



From C.K.Cline and M. Blann, Nucl. Phys.**A172**(1971)225.

Integrated emission rates - I

The solution to the master equation can be written in vector form as

$$\vec{P}(t) = \exp\left[-\Lambda^{-1} t\right] \vec{P}_{0,} \qquad \text{with} \qquad P_0(n) = \sigma_{abs}\delta_{p,2}\delta_{h,1},$$

where the matrix Λ^{-1} is given by

$$\left(\Lambda^{-1}\right)_{nm} = \lambda(n)\,\delta_{m,n} - \lambda_{-}(n+2)\,\delta_{m,n+2} - \lambda_{+}(n-2)\,\delta_{m,n-2}$$

The time-integrated emission spectrum is

$$\frac{d\sigma}{d\varepsilon} = \sum_n \int_0^\infty \frac{d\lambda_e}{d\varepsilon}(n,\varepsilon)\,P(n,t)\,dt = \sum_{n,m} \frac{d\lambda_e}{d\varepsilon}(n,\varepsilon)\,\underbrace{\Lambda_{n,m}P_0(m)}_{\tau_n\,\sigma_{abs}}$$

Integrated emission rates - II

When the emission rates are very small compared to the transition rates, the smallest eigenvalue of the matrix τ_0^{-1} tends to

$$\tau_0^{-1} \to \sum_n \lambda_e(n)\,\omega(n,E) \quad \text{and} \quad \sum_m \Lambda_{nm} P_0(m) \to \tau_0\,\omega(n,E)\,\sigma_{abs}$$

The emission spectrum is then the equilibrium one

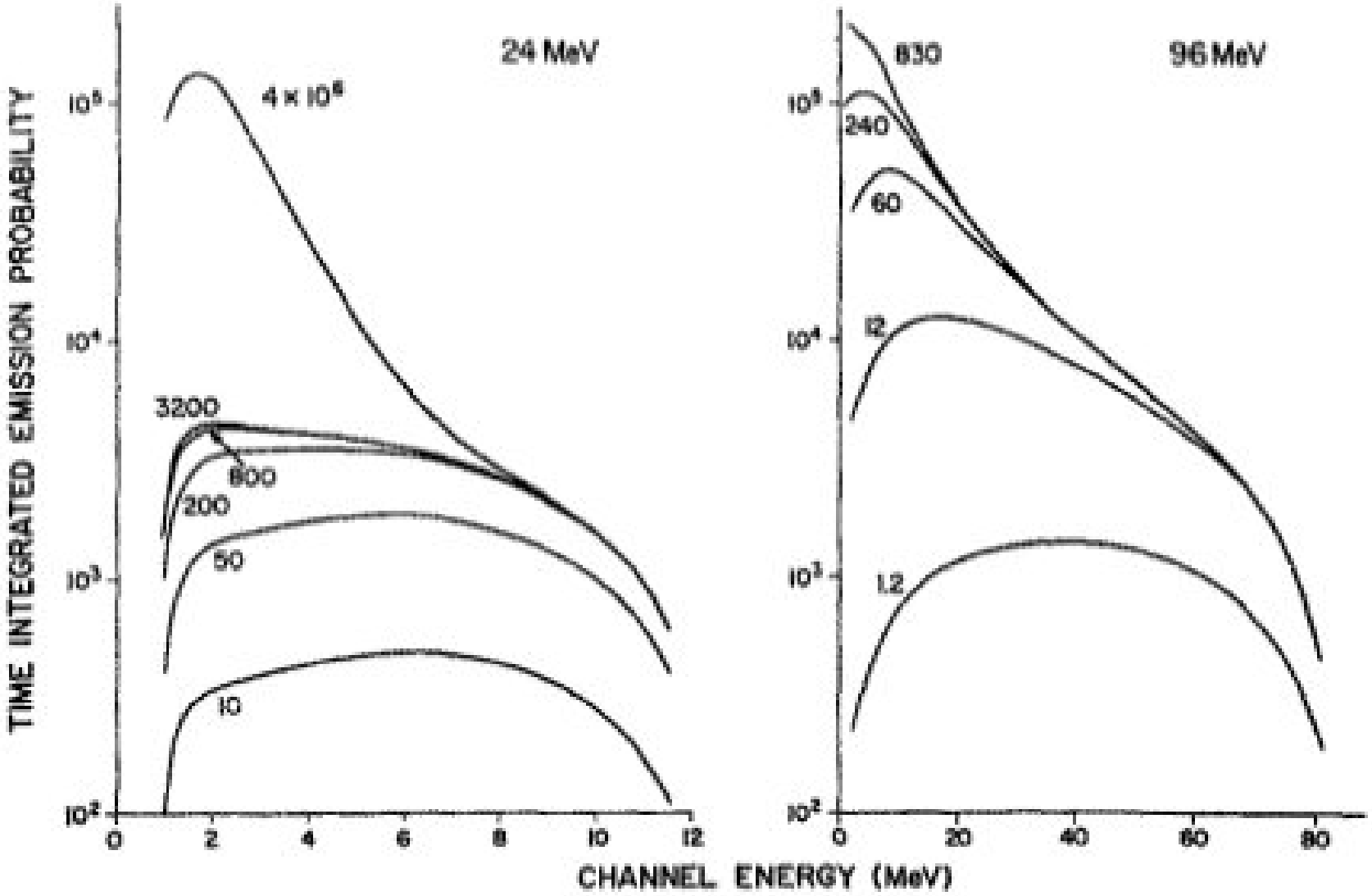
$$\frac{d\sigma}{d\varepsilon} = \sigma_{abs} \sum_n \frac{d\lambda_e}{d\varepsilon}(n,\varepsilon)\,\omega(n,E) \Big/ \sum_n \lambda_e(n)\,\omega(n,E)$$

since

$$\sum_n \frac{d\lambda_e}{d\varepsilon}(n,\varepsilon)\,\omega(n,E) = (2s+1)\frac{\mu\varepsilon\sigma(\varepsilon)}{\pi^2\hbar^3} \sum_n \omega(n-1,U)$$

$$= (2s+1)\frac{\mu\varepsilon\sigma(\varepsilon)}{\pi^2\hbar^3}\,\omega_{tot}(U)$$

Integrated emission rates - III



From C.K.Cline and M. Blann, Nucl. Phys.**A172**(1971)225.

The never-come-back approximation

Preequilibrium spectra are determine by the integrated solution to the master equation, which we can write as

$$\Lambda^{-1}\vec{\tau} = \vec{P}_0 \quad \text{with} \quad P_0(n) = \delta_{p,2}\delta_{h,1}$$

In component form, this can be written as

$$\lambda(n)\,\tau(n) - \lambda_+(n-2)\,\tau(n-2) - \lambda_-(n+2)\,\tau(n+2) = \delta_{n,3}$$

As we have seen, $\lambda_{n-} << \lambda_{n+}$ in the early stages of a reaction. If we neglect the λ_{n-}, we have

$$\begin{aligned}
\lambda(3)\tau(3) &= 1 \\
\lambda(5)\tau(5) - \lambda_+(3)\tau(3) &= 0 \\
\lambda(7)\tau(7) - \lambda_+(5)\tau(5) &= 0 \\
&\vdots
\end{aligned}
\quad \Rightarrow \quad
\begin{aligned}
\tau(3) &= 1/\lambda(3) \\
\tau(5) &= \lambda_+(3)\tau(3)/\lambda(5) \\
\tau(7) &= \lambda_+(5)\tau(5)/\lambda(7) \\
&\vdots
\end{aligned}$$

This is continued up to an “equilibrium“ value of the exciton number – n_{eq}. The remaining probability is assumed to decay from equilibrium.

Gamma emission

Preequilibrium photon emission can be included by using the Brink-Axel hypothesis. An n exciton state can decay to an n or an n-2 exciton state by emission of a dipole photon (GDR).

The differential emission rate is

$$\frac{d\lambda_{e\gamma}}{d\varepsilon}(n,\varepsilon) = \frac{e^2\sigma_\gamma(\varepsilon)}{\pi^2\hbar^3c^2}\sum b(k\to n,\varepsilon)\frac{\omega(k,E-\varepsilon)}{\omega(n,E)}$$

To be consistent with equilibrium emission, we must have

$$b(n\to n+2,\varepsilon)+b(n\to n,\varepsilon)=1$$

We can argue that

$$b(n\to n,\varepsilon)\propto n \quad \text{and} \quad b(n\to n+2,\varepsilon)\propto \omega(p=1,h=1,\varepsilon)/g$$

which imply that

$$\sum b(k\to n,\varepsilon)\omega(k,E-\varepsilon) = \frac{\omega(2,\varepsilon)\omega(n-2,E-\varepsilon)}{\omega(2,\varepsilon)+g(n-2)} + \frac{gn\,\omega(n,E-\varepsilon)}{\omega(2,\varepsilon)+gn}$$

E. Beták and J. Dobes, Phys. Lett. **84B** (1979) 368.
J.M. Akkermans and H. Gruppelaar, Phys. Lett. **157B** (1985) 95.

Protons and neutrons

We have not distinguished protons and neutrons up to this point, although they have important differences, such as the Coulomb inhibition of proton emission and different separation energies.

A simple way of taking these differences into account is through their emission rates. We take for neutrons

$$\frac{d\lambda_{e\nu}}{d\varepsilon}(n,\varepsilon) = (2s+1)\frac{\mu\varepsilon\sigma_{\nu}(\varepsilon)}{\pi^2\hbar^3}R_{\nu}(n)\frac{\omega(n-1,E-\varepsilon-B_{\nu})}{\omega(n,E)}$$

and for protons

$$\frac{d\lambda_{e\pi}}{d\varepsilon}(n,\varepsilon) = (2s+1)\frac{\mu\varepsilon\sigma_{\pi}(\varepsilon)}{\pi^2\hbar^3}R_{\pi}(n)\frac{\omega(n-1,E-\varepsilon-B_{\pi})}{\omega(n,E)}$$

where $R_x(n)$ is the fraction of particles of type x (π or ν) in exciton class n.

The emission rate that enters the master equation is

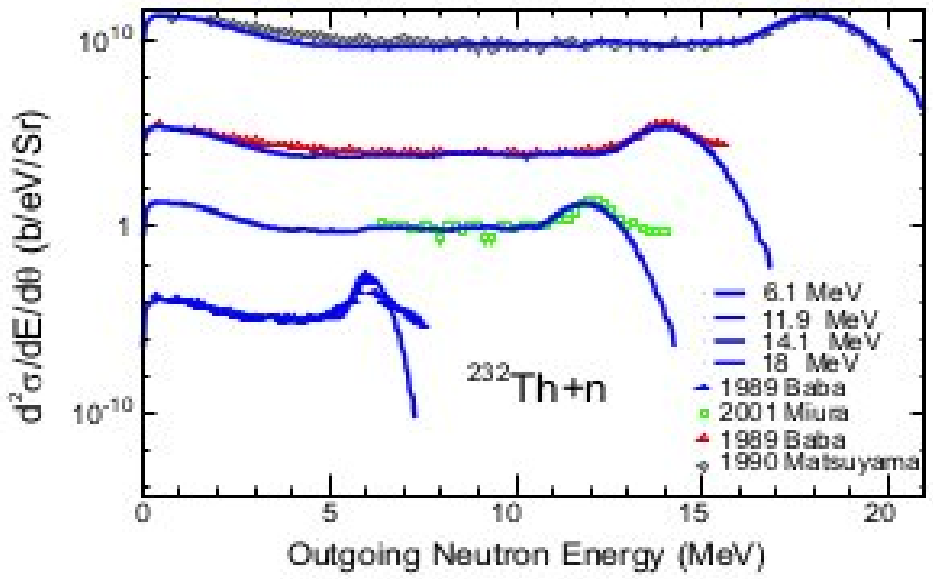
$$\lambda_e(n) = \lambda_{e\nu}(n) + \lambda_{e\pi}(n) = \int \left(\frac{d\lambda_{e\nu}}{d\varepsilon}(n,\varepsilon) + \frac{d\lambda_{e\pi}}{d\varepsilon}(n,\varepsilon) \right) d\varepsilon$$

PCROSS

The PCROSS subroutine in EMPIRE performs exciton model calculations. PCROSS

- uses the never-come-back approximation;
- distinguishes protons and neutrons through their emission rates;
- includes pre-equilibrium gamma emission;
- includes cluster emission (to be discussed later).

The calculation shown here also takes into account direct contributions through CC+DWBA calculations.



From NDS **108** (2007) 2655.

The two component exciton model - I

Modified emission rates describe a good part of the difference between proton and neutron preequilibrium emission. However, they cannot take into account differences in the transitions rates between protons and neutrons. Nor can they correct for the fact that the sum of single-component exciton densities of states does not produce the correct total density of states.

The two-component model corrects these deficiencies. The master equation is much more complicated, however. We now have

$$\begin{aligned}\frac{dP(n_\pi,n_\nu)}{dt} &= \lambda_{\pi-}(n_\pi+2,n_\nu)P(n_\pi+2,n_\nu)+\lambda_{\nu-}(n_\pi,n_\nu+2)P(n_\pi,n_\nu+2)\\ &+\lambda_{\pi\nu 0}(n_\pi+2,n_\nu-2)P(n_\pi+2,n_\nu-2)\\ &+\lambda_{\nu\pi 0}(n_\pi-2,n_\nu+2)P(n_\pi-2,n_\nu+2)\\ &+\lambda_{\pi+}(n_\pi-2,n_\nu)P(n_\pi-2,n_\nu)+\lambda_{\nu+}(n_\pi,n_\nu-2)P(n_\pi,n_\nu-2)\\ &-\lambda(n_\pi,n_\nu)P(n_\pi,n_\nu)\end{aligned}$$

where $n_\pi = p_\pi + h_\pi$ and $n_\nu = p_\nu + h_\nu$

C. Kalbach, Phys. Rev. C **33** (1986) 818.
A. J. Koning and M. Duijvestijn, Nucl. Phys. A **744** (2004) 15.

The two component exciton model - II

The exciton densities become

$$\omega(p_\pi, h_\pi, p_\nu, h_\nu, E) = \frac{g_\pi^{n_\pi} g_\nu^{n_\nu} \left(gE - A_{p_\pi,h_\pi,p_\nu,h_\nu}\right)^{n-1}}{p_\pi! h_\pi! p_\nu! h_\nu! (n-1)!} f(p,h,E)$$

where

$$A_{p_\pi,h_\pi,p_\nu,h_\nu} = \frac{p_\pi(p_\pi-1)+h_\pi(h_\pi-1)}{4g_\pi} + \frac{p_\nu(p_\nu-1)+h_\nu(h_\nu-1)}{4g_\nu}$$

and the function f(p,h,E) depends on the total number of holes.

The transition rates now include more collision possibilities as well,

$$\lambda_{\pi+}(n)\omega(n,E) = \lambda_{\pi-}(n+2)\omega(n+2,E) =$$

$$= \frac{2\pi}{\hbar}\int_0^E d\varepsilon \left(|M_{\pi\pi}|^2 \omega(2,1,0,0,\varepsilon)\omega(1,0,0,0,\varepsilon)\omega(p_\pi-1,h_\pi,p_\nu,h_\nu,E-\varepsilon) \right.$$
$$+|M_{\pi\pi}|^2 \omega(1,2,0,0,\varepsilon)\omega(0,1,0,0,\varepsilon)\omega(p_\pi,h_\pi-1,p_\nu,h_\nu,E-\varepsilon)$$
$$+|M_{\pi\nu}|^2 \omega(1,1,1,0,\varepsilon)\omega(0,0,1,0,\varepsilon)\omega(p_\pi,h_\pi,p_\nu-1,h_\nu,E-\varepsilon)$$
$$\left. +|M_{\pi\nu}|^2 \omega(1,1,0,1,\varepsilon)\omega(0,0,0,1,\varepsilon)\omega(p_\pi,h_\pi,p_\nu,h_\nu-1,E-\varepsilon) \right)$$

Angular momentum - I

The exciton model can be generalized to conserve angular momentum as well as energy. The master equation is identical to those we have seen before. We have (in the case in which we don't distinguish protons and neutrons)

$$\frac{dP(n,J)}{dt} = \lambda_-(n+2,J)\,P(n+2,J) + \lambda_+(n-2,J)\,P(n-2,J) - \lambda(n,J)\,P(n,J)$$

where

$$\lambda(n,J) = \lambda_-(n,J) + \lambda_+(n,J) + \lambda_e(n,J)$$

The exciton level densities are written in terms of the densities of states as

$$\rho(p,h,E,J) = \omega(p,h,E)\,R_n(J)$$

where the spin distribution is given by

$$R_n(J) = \frac{2J+1}{\sqrt{\pi}(2\sigma_n^2)^{3/2}} \exp\left(-\frac{(J+1/2)^2}{2\sigma_n^2}\right)$$

The spin cutoff parameter is well parametrized by

$$\sigma_n^2 = (0.24 + 0.0038E)A^{2/3}\,n$$

Angular momentum - II

The transition rates can be written in a form analogous to the earlier one, but in terms of level densities and average *reduced* matrix elements, as

$$\lambda_+(n,E,J)\rho(n,E,J) = \lambda_-(n+2,E,J)\rho(n+2,E,J) =$$

$$= \frac{2\pi}{\hbar} \sum_{\vec{j}+\vec{J}'=\vec{J}} |\tilde{M}_j|^2 \int_0^E d\varepsilon \, (\rho(2,1,\varepsilon,j)\rho(1,0,\varepsilon,j)\rho(p-1,h,E-\varepsilon,J')$$

$$+ \rho(1,2,\varepsilon,j)\rho(0,1,\varepsilon,j)\rho(p,h-1,E-\varepsilon,J'))$$

The emission widths are now written in terms of the transmission coefficients as

$$\frac{d\lambda_{ex}}{d\varepsilon}(n,\varepsilon,J) = \frac{R_x(n)}{h} \sum_{\vec{l}+\vec{s}+\vec{J}'=\vec{J}} T_{xl}(\varepsilon) \frac{\rho(n-1,E-\varepsilon-B_x,J')}{\rho(n,E,J)}$$

where x can be π or ν.

The code DEGAS by E. Beták and P. Oblozinský uses the angular momentum conserving exciton model.

V.A. Plujko, Yad.Fiz. **27** (1978) 1175.

X. Shi, H. Gruppelaar, J.M. Akkermans, Nucl. Phys. A **466** (1987) 333.

Multiple emission

Secondary pre-equilibirum emission becomes important above about 50 Mev and higher pre-equilibrium emissions grow in importance as the incident particle energy increases. Their effects can be seen in:

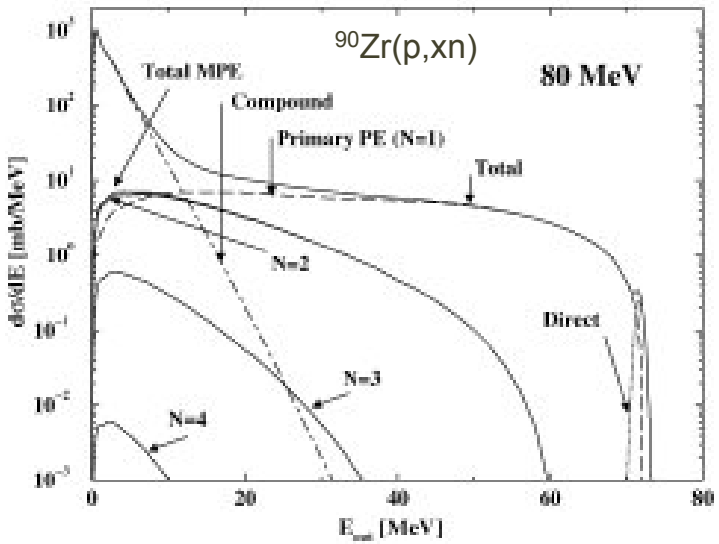
1) emission spectra, in which the multiple emission contributes most at energies just above the equilibrium peak;

2) residual populations, which do not extend as far down the decay chain due to the extra energy carried by the pre-equilibrium particles.

The calculation of secondary emission is conceptually straight forward but cumbersome. The population of the A-1 nucleus after the first emission is given by

$$P_1(n-1, E-\varepsilon-B) = \frac{d\lambda_e}{d\varepsilon}(n,\varepsilon)\tau_n$$

These probabilities define the initial conditions for the solution of the master equation of the p=h=n/2 chain of exciton classes.



A. J. Koning and M. Duijvestijn, Nucl. Phys. A **744** (2004) 15.

The generalized exciton model - I

Here, the evolution of the reaction is described in terms of the exciton number n and the direction of the *incident* nucleon Ω. The transition rates are assumed to be factorizable into the usual transition rates times an angular part proportional to the free nucleon-nucleon angular distribution,

$$\lambda_{n\leftarrow m}(\Omega \leftarrow \Omega') = \lambda_{n\leftarrow m} G(\Omega,\Omega') = \lambda_{n\leftarrow m} \frac{1}{\sigma_{NN}} \frac{d\sigma_{NN}}{d\Omega}$$

The master equation becomes

$$\frac{dP(n,\Omega)}{dt} = \sum_{m=n-2}^{n+2} \lambda_{n\leftarrow m} \int d\Omega' G(\Omega,\Omega') P(m,\Omega') - \lambda(n) P(n,\Omega)$$

where

$$\lambda(n) = \sum_{m=n-2}^{n+2} \lambda_{m\leftarrow n} + \lambda_e(n)$$

The emission rate is assumed to have its usual form and the particle is assumed to be emitted in the direction Ω.

G. Mantzouranis, H.A. Weidenmüller, D. Agassi, Z. Phys. A **276** (1976) 145.
J.M. Akkermans, H. Gruppelaar, G. Reffo, Phys. Rev. C **22** (1980) 73.

The generalized exciton model - II

The scattering kernel depends on the angle between Ω and Ω', so that

$$G(\Omega,\Omega') = \sum_{l=0} \mu_l Y_{lm}(\Omega) Y^*_{lm}(\Omega') \qquad \text{with} \quad \mu_0 = 1$$

Due to the axial symmetry of the problem, the master equation can then be expanded in terms of the Legendre polynomials as

$$\frac{dP(n,l)}{dt} = \mu_l \left(\lambda_+(n-2)P(n-2,l) + \lambda_0(n)P(n,l) + \lambda_-(n+2)P(n+2,l)\right) - \lambda(n)P(n,l)$$

where

$$P(n,\Omega) = \sum_{l=0} P(n,l) P_l(\cos\theta)$$

After solving the set of equations, the emission spectrum can be obtained as

$$\frac{d^2\sigma}{d\varepsilon d\Omega} = \sigma_{abs} \sum_{n=3,5,\ldots} \lambda_e(n)\tau(n,\Omega) \quad \text{where} \quad \tau(n,\Omega) = \int_0^\infty P(n,\Omega,t)dt$$

The generalized exciton model tends to underestimate the spectrum at backwards angles. It only describes the “leading”particle.

The Kalbach systematics

Kalbach observed that the pre-equilibrium/equilibrium double differential spectrum consists of two parts:

1) a forward-peaked continuum contribution,

$$\frac{d^2\sigma}{d\varepsilon d\Omega} = \frac{1}{4\pi}\frac{d\sigma_{MSD}}{d\varepsilon}\frac{2a}{e^a - e^{-a}}\exp(a\cos\theta)$$

2) and a bound-state contribution that is symmetric about 90°.

$$\frac{d^2\sigma}{d\varepsilon d\Omega} = \frac{1}{4\pi}\frac{d\sigma_{MSC}}{d\varepsilon}\frac{a}{e^a - e^{-a}}[\exp(a\cos\theta) + \exp(-a\cos\theta)]$$

Combining the two gives

$$\frac{d^2\sigma}{d\varepsilon d\Omega} = \frac{1}{4\pi}\frac{d\sigma}{d\varepsilon}\frac{a}{\sinh(a)}[\cosh(a\cos\theta) + f_{MSD}\sinh(a\cos\theta)]$$

where the continuum fraction f_{MSD} must be determined separately.

Kalbach obtained an excellent description of many pre-equilibrium angular distributions by parametrizing the coefficient a in terms of the incident and exit particle energies.

C. Kalbach, F.M. Mann, Phys. Rev. C **23** (1981) 112.
C. Kalbach, Phys. Rev. C **37** (1988) 2350.

The hybrid model

The hybrid model is similar to an exciton model in which the internal transitions are associated explicitly with nucleon-nucleon scattering rather than with two-body matrix elements. It gives for the probability of finding a particle of type x (π or ν) with energy ε

$$P_x(\varepsilon) = \sum_{n=3,5,\ldots}^{n_{eq}} R_x(n)\, g \frac{\omega(n-1, E-\varepsilon-B)}{\omega(n,E)} \frac{\lambda_e(\varepsilon)}{\lambda_e(\varepsilon)+\lambda_+(\varepsilon)} D_n$$

and for the emission spectrum

$$\frac{d\sigma_x}{d\varepsilon} = P_x(\varepsilon)\sigma_{abs}$$

where the transition rate is given in terms of the mean free path MFP as

$$\lambda_+(\varepsilon) = \frac{v}{MFP(\varepsilon)} = \rho_0 \langle \sigma(\varepsilon) \rangle \sqrt{\frac{2(\varepsilon+V)}{m}}$$

and the emission width as

$$\lambda_{ex}(\varepsilon) = (2s+1)\frac{\mu\varepsilon\sigma_x(\varepsilon)}{\pi^2\hbar^3 g}$$

The geometry-dependent hybrid model

The geometry-dependent hybrid model improves the agreement of the hybrid model with experimental data by taking into account effects of the nuclear surface. It first associates a value of the angular momentum with the impact parameter using the standard rule,

$$kb = l + 1/2$$

An average density is calculated in terms of the integral of a Wood-Saxon density on a straight line trajectory with that impact parameter

$$\bar{\rho}_0(l) = \left\langle \frac{\rho_0}{1 + \exp[(\sqrt{b^2 + z^2} - R_0)/a]} \right\rangle$$

The average density is used to determine the mean free path, as well as the Fermi energy, which determines the depth V of the potential and the limit to hole excitation, which enters the density of states. The spectrum is calculated as

$$\frac{d\sigma_x}{d\varepsilon} = \frac{\pi}{k^2} \sum_l (2l+1) T_l P_x(l, \varepsilon)$$

The transition rate and the optical potential

The mean free path is determined by the in-medium scattering cross section as

$$MFP(\varepsilon) = \frac{1}{\rho_0 \langle \sigma(\varepsilon) \rangle}$$

where ρ_0 is the nucleon density.

When the potential is complex, a propagating wave decays as $e^{-2k_i r}$ where

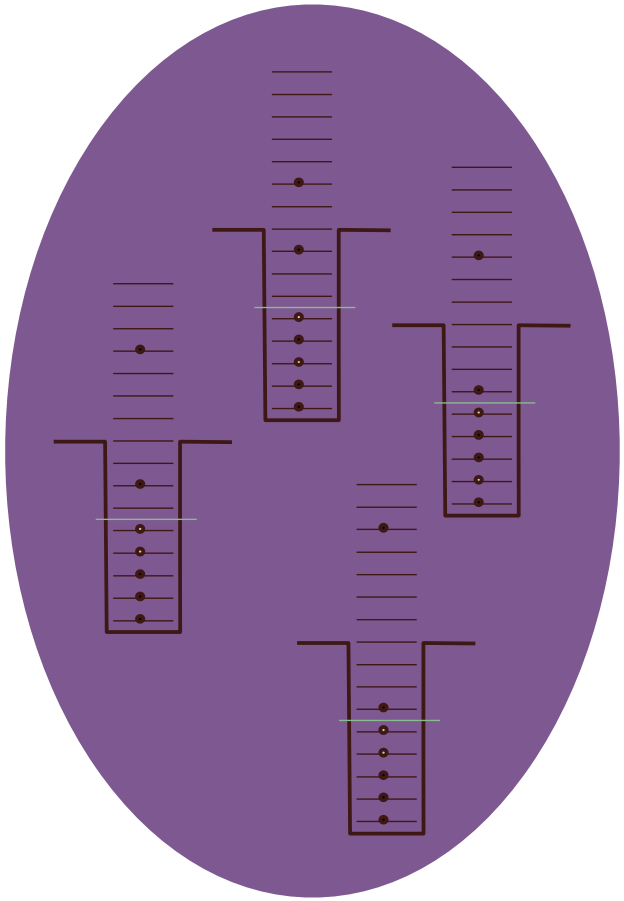
$$k_i = \mathrm{Im}\left[\frac{\sqrt{2m(\varepsilon + V + iW)}}{\hbar}\right] \approx \frac{W}{\hbar v}$$

so that we can also write

$$MFP(\varepsilon) = \frac{\hbar v}{2W} \quad \text{and} \quad \lambda_+(\varepsilon) = \frac{v}{MFP(\varepsilon)} = \frac{2W}{\hbar}$$

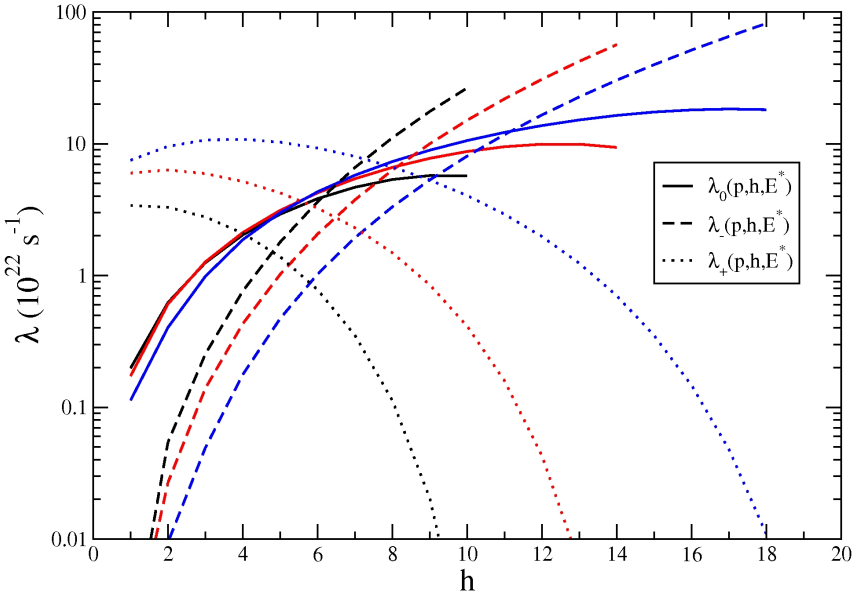
A problem with the exciton model

- The standard exciton model assumes that the configurations with the same number of excitons are equally probable;
- Bisplinghoff showed that this is not automatic for transitions beyond those to the 2p-1h class;
- Equilibration among the confiurations within a class would make this the case;
- The assumption of equilibrium would also permit the use of the exciton densities of states and transition densities, which greatly simplify the calculation.
- Is the assumption of equilibrium justified?
- This can be verified by comparing the transition rate that does not change the number of excitons - and which mixes the configurations – with the others.



J. Bisplinghoff, Phys. Rev. **C33** (1986) 1569.

Exciton model transition rates

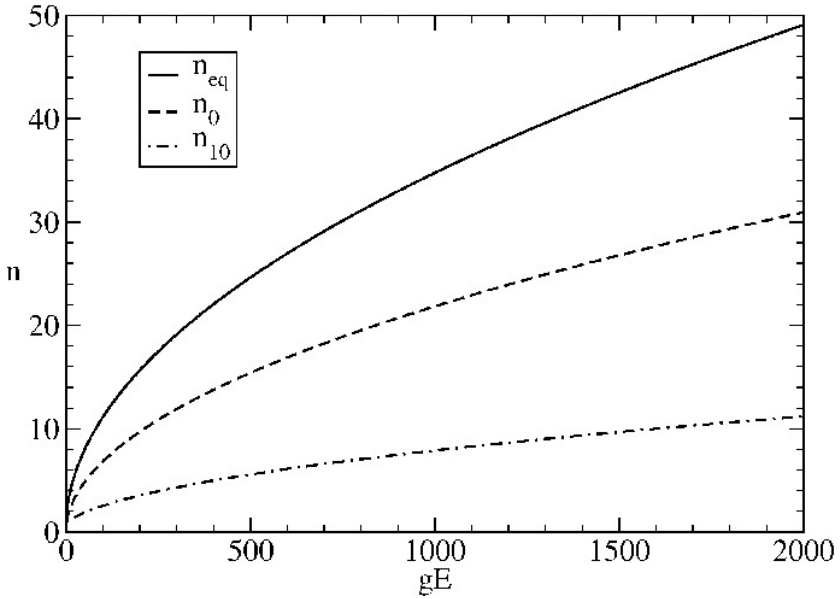


Transition rates for nucleon + ^{40}Ca

Incident energies of
25, 50 and 100 MeV.

or

gE = 75, 150, 300



We can define an effective exciton number for equilibrium, n_{eq}, as

$$n_{eq} : \lambda_+(n_{eq}, E) = \lambda_-(n_{eq}, E)$$

and for equilibration within an exciton class, n_0, as

$$n_0 : \lambda_+(n_0, E) = \lambda_0(n_0, E)$$

BVC, J. E. Escher, M. S. Hussein, . Phys. G41 (2014) 094003.

Monte Carlo simulations

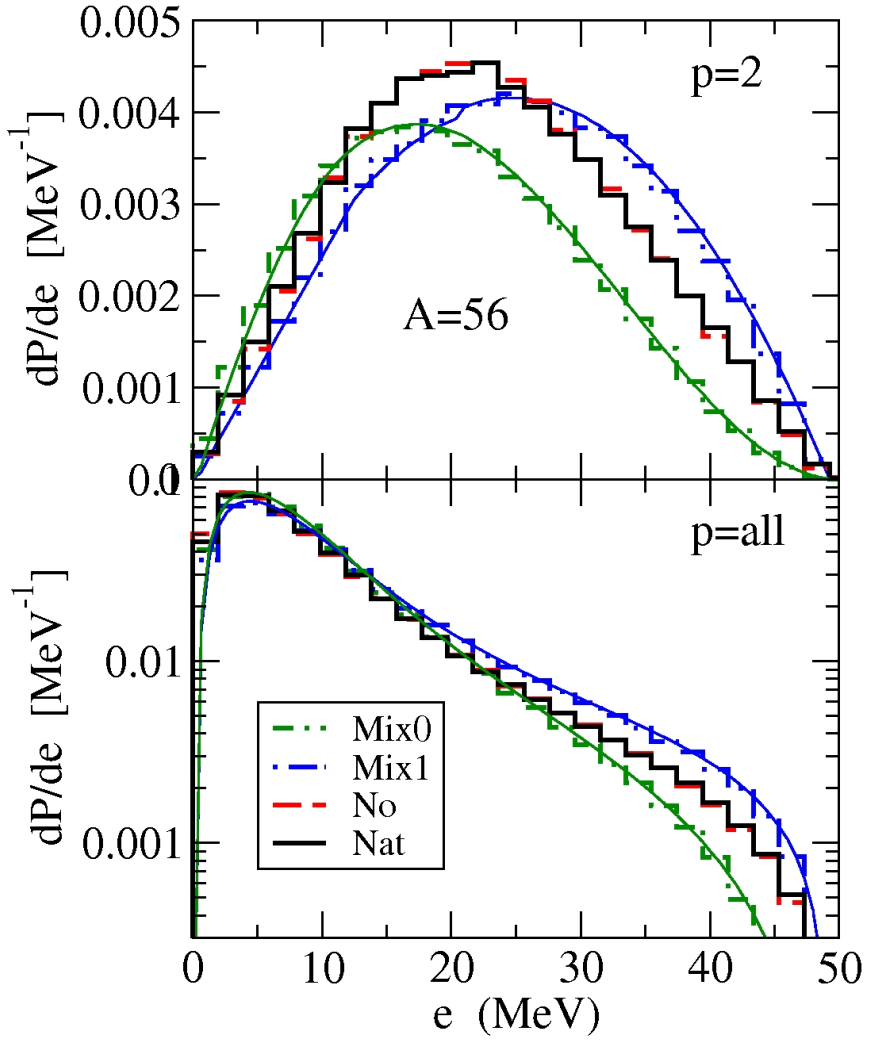
Simulations with:
- No mixing – no transitions with $\Delta n=0$;
- Natural mixing – $\Delta n=0$ transitions with same weight as others;
-Complete mixing – $\Delta n=0$ transitions 1000 times others.

•The complete-mixing and exciton model results are almost identical;

•The no-mixing and 'natural' model results are also almost identical;

•Complete-mixing and no-mixing results differ - the exciton model requires complete mixing;

•The fixed-hole and free-hole results are very different.



Energy spectrum of first emitted nucleon in nucleon + ^{56}Fe at an incident energy of 50 MeV.

C. A. Soares Pompeia and B. V. Carlson, Phys. Rev. **C74** (2004) 054609.

The hybrid Monte Carlo simulation (HMS) model

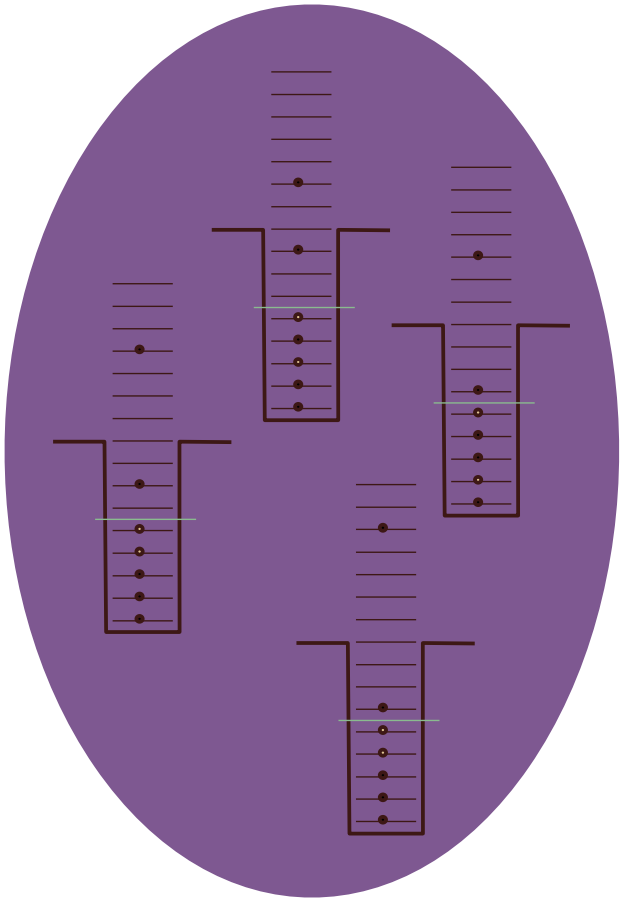
- The HMS model ignores transitions between configurations with the same number of excitons – no mixing;

- As in the geometry-dependent hybrid model, the $\Delta n=2$ transition rate is calculated using the geometry-dependent in-medium cross section;

- Protons and neutrons are distinguished as in a two-component model.

- Transitions and emission from each particle and hole in a configuration are treated independently;

- For a nucleon + ^{40}Ca at 100 MeV, 10^9 configurations versus 20 exciton classes – Monte Carlo simulation.



M. Blann, Phys. Rev. C **54** (1996) 1341.

The Monte Carlo procedure

0) Initially, the incident nucleon is chosen to scatter, creating a 2p-1h configuration.

1) In subsequent steps, a table of emission rates (particles) and transitions rates (particles and holes) is associated with the unit interval. The drawing of a random number can then be associated with the random choice of emission or collison of a well-defined particle or hole.

2) If a particle is chosen to escape,
a) its properties are accumulated in the table of emitted particles
b) the particle is eliminated from the rate table.

3) If an exciton is chosen to scatter,
a) first a collision partner and then its energy are drawn randomly. (If the colliding exciton is a particle, the partner will be the final hole. If it is a hole, the partner is the final particle.)
b) the final energy of the colliding exciton is drawn randomly and the final energy of the collision partner is determined by energy conservation.
c) the emission and transition rates of the new excitons are calculated and stored in the rate table, if they are not bound.

The Monte Carlo sampling I

- The scattering partner of a given particle or hole is chosen according to the relative nucleon-nucleon cross sections. For example, if the initial particle or hole is of neutron type, then the probability of the partner being a neutron will be

$$P_{nn} = \frac{(A-Z)\sigma_{nn}}{(A-Z)\sigma_{nn} + Z\sigma_{np}} \qquad \text{with} \qquad P_{np} = 1 - P_{nn}$$

- To obtain the hole energy in a 1p->2p1h collision, we use the exciton phase space integral

$$\begin{aligned}\omega(3,\varepsilon_{p0}) &= \frac{g^3}{2}\int d\varepsilon_h d\varepsilon_{p1} d\varepsilon_{p2}\,\theta(V-\varepsilon_h)\,\delta(\varepsilon_{p0}-\varepsilon_h-\varepsilon_{p1}-\varepsilon_{p2}) \\ &= \frac{g^3}{2}\int_0^{\min(\varepsilon_{p0},V)} d\varepsilon_h \int_0^{\varepsilon_{p0}-\varepsilon_h} d\varepsilon_{p1}\end{aligned}$$

to obtain its probability distribution

$$P(\varepsilon_h) = \frac{2(\varepsilon_{p0}-\varepsilon_h)}{(2\varepsilon_{p0}-\varepsilon_{hmax})\varepsilon_{hmax}} \qquad \text{where} \quad \varepsilon_{hmax} = \min(\varepsilon_{p0}, V)$$

The Monte Carlo sampling I

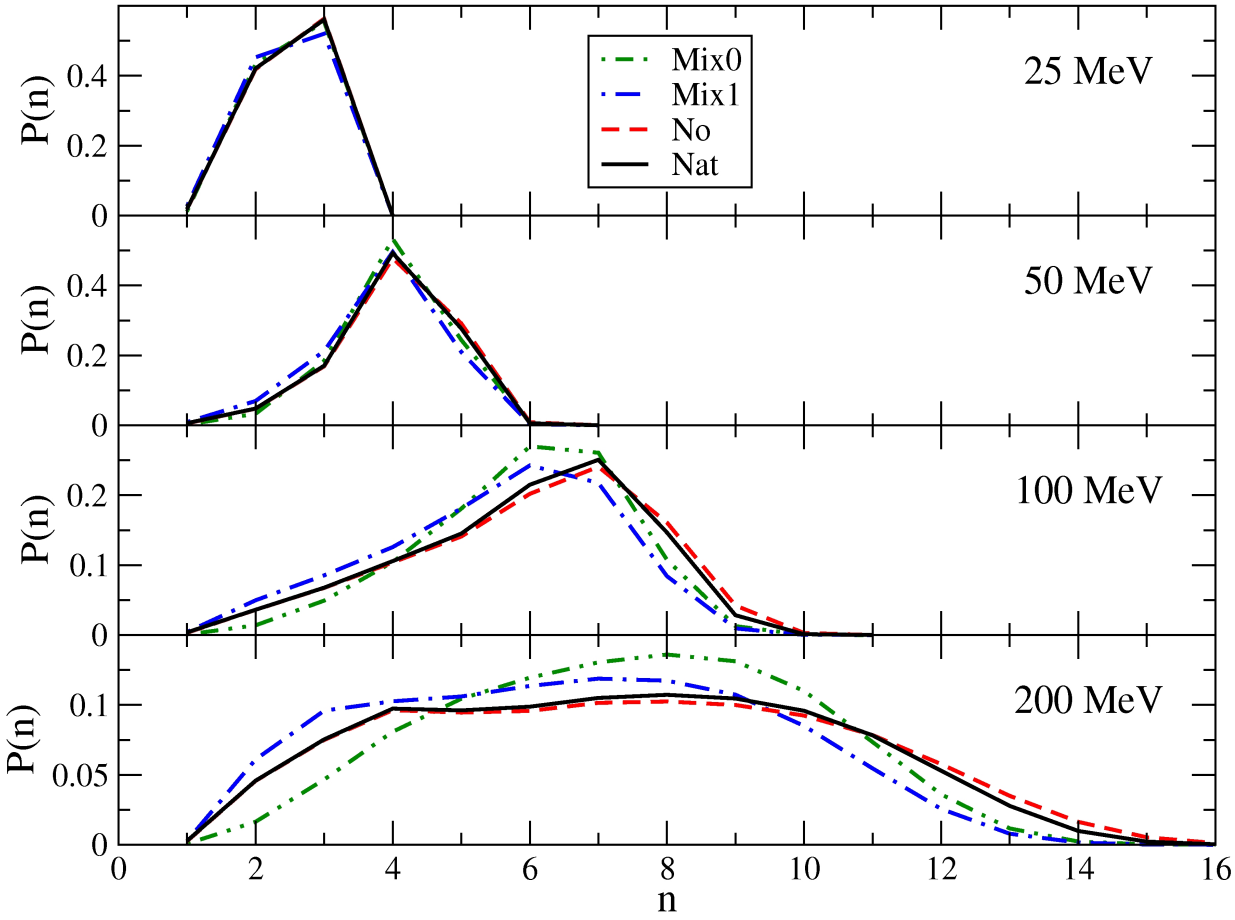
Once the hole energy is determined, one of the final particles can be drawn from a uniform distribution, since

$$P(\varepsilon_{p1}) = \frac{1}{\varepsilon_{p0} - \varepsilon_h} \qquad \text{with} \qquad \varepsilon_{p1,max} = \varepsilon_{p0} - \varepsilon_h$$

We have assumed a constant-spacing single particle density of states in this example. The densities can also be determined using Fermi gas single-particle densities. Both options are in the code.

The HMS uses experimental bindng energies and takes into account scattering and emission of neutrons and protons. The Monte Carlo sampling allows as many transitions and emissions as are necessary for the remaining degrees of freedom to be bound. It also facilitates the calculation of residual populations, recoil spectra and particle angular distributions. We will discuss the last of these in more detail later.

Multiple emission



Distribution of number of emitted nucleons from nucleon + ^{40}Ca at incident energies of 25, 50, 100 and 200 MeV.

Linear momentum densities - I

Particle-hole densities in which both energy and linear momentum are defined can be written as

$$\omega(p,h,E,\vec{K}) = \frac{1}{p!h!}\int \prod_{i=1}^{p}\omega_1(\vec{k}_i)\theta(k_i-k_F)d^3k_i \prod_{j=1}^{h}\omega_1(\vec{k}_j)\theta(k_F-k_j)d^3k_j \times\delta\left(E-\sum_{i=1}^{p}\varepsilon_i+\sum_{j=1}^{h}\varepsilon_j\right)\delta\left(\vec{K}-\sum_{i=1}^{p}\vec{k}_i+\sum_{j=1}^{h}\vec{k}_j\right)$$

where

$$\omega_1(\vec{k}) = \begin{cases} \frac{A}{\frac{4\pi}{3}k_F^3} & \text{Fermi-gas levels} \\ \frac{g}{4\pi mk} & \text{equidistant levels} \end{cases}$$

This density can be calculated explicitly only for low exciton number but it can be well-approximated statistically for larger exciton numbers. We write it as a product of the conventional density and a momentum-dependent term,

$$\omega(p,h,E,\vec{K}) = \omega(p,h,E)\,M(p,h,E,\vec{K})$$

M.B. Chadwick, P. Oblozinský, Phys. Rev. C **46** (1992) 2028.

Linear momentum densities - II

When the exciton number is large, we expect the sum of randomly oriented exciton momenta to be zero. We also expect that we can apply the central limit theorem to obtain

$$M(p,h,E,\vec{K}) = \frac{1}{(2\pi)^{3/2}\sigma^3}\exp(-K^2/2\sigma^2)$$

The cutoff parameter σ^2 is given by the sum of the average squared projection of the exciton momentum,

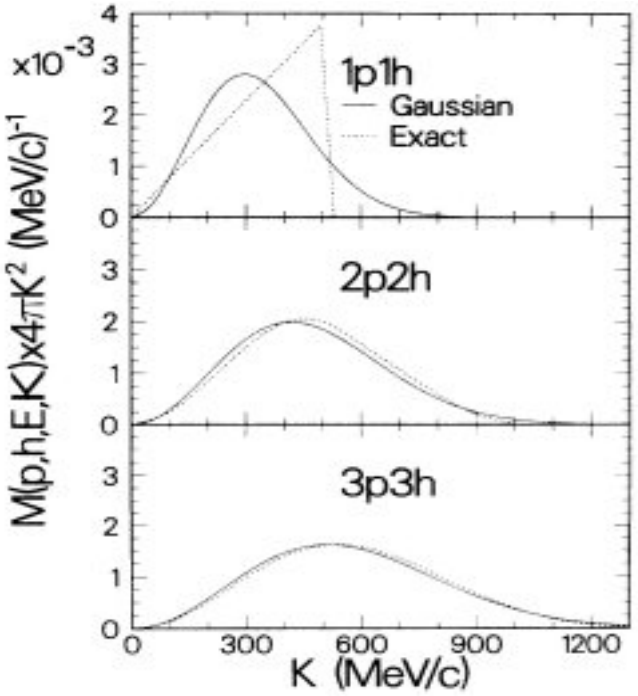
$$\sigma^2 = \sum_{i=1}^{n}\left\langle (k_i^{proj})^2 \right\rangle$$

with

$$\left\langle (k_i^{proj})^2 \right\rangle = \frac{1}{4\pi}\int (k_i\cos\theta_i)^2 = \frac{k_i^2}{3}$$

so that

$$\sigma^2 = \frac{2m\varepsilon_{av}}{3}n$$



From M.B. Chadwick, P. Oblozinský, Phys. Rev. C **46** (1992) 2028.

Linear momentum and the Kalbach systematics

When the exciton model is extended to take into account linear momentum, the differential emission rate becomes

$$\frac{d^2\lambda_e}{d\varepsilon d\Omega}(n,\varepsilon,\Omega) = (2s+1)\frac{\mu\varepsilon\sigma(\varepsilon)}{\pi^2\hbar^3}\frac{\omega(n-1,U,\vec{K}-\vec{k})}{\omega(n,E,\vec{K})}$$

where the particle momentum is in the direction Ω and $\varepsilon = k^2/2m$.
We rewrite this as

$$\frac{d^2\lambda_e}{d\varepsilon d\Omega}(n,\varepsilon,\Omega) = \frac{d\lambda_e}{d\varepsilon}(n,\varepsilon)\frac{M(n-1,U,\vec{K}-\vec{k})}{M(n,E,\vec{K})}$$

and use

$$(\vec{K}-\vec{k})^2 = K^2 + k^2 - 2Kk\cos\theta$$

to approximate this as

$$\frac{d^2\lambda_e}{d\varepsilon d\Omega}(n,\varepsilon,\Omega) = \frac{d\lambda_e}{d\varepsilon}(n,\varepsilon)\frac{1}{4\pi}\frac{a_n}{\sinh(a_n)}\exp(a_n\cos\theta)$$

with $$a_n = \frac{Kk}{\sigma_n^2} = \frac{3Kk}{2(n-1)m\varepsilon_{av}}$$

M.B. Chadwick, P. Oblozinský, Phys. Rev. C **50** (1994) 2490.

The double differential HMS – DDHMS - I

The HMS model can easily be extended to calculate double differential emission spectra using linear momentum densities.

This is done by randomly drawing values for each of the particle/hole angles in a scattering process after the energies have been drawn.

For example,

1) after the hole energy in a 2p-1h process has been drawn, the angle θ_h of the hole momentum relative to the direction of the initial particle is drawn from the probability distribution

$$P_3(\cos\theta_h) = \frac{a_3}{\sinh(a_3)}\exp(a_3\cos\theta_h)$$

and its azimuthal angle π_h is drawn from a uniform distribution between 0 and 2π.

The momentum of the remaining 2p distribution is then calculated using momentum conservation.

M. Blann, M. B. Chadwick, Phys. Rev. C **57** (1998) 233.

The double differential HMS – DDHMS - II

2) after the energy of the first of the two final particles has been drawn, its angle θ_{p1} relative to the remaining momentum is drawn from the corresponding two-exciton probability distribution,

$$P_2(\cos\theta_{p1}) = \frac{a_2}{\sinh(a_2)}\exp(a_2\cos\theta_{p1})$$

and its azimuthal angle θ_{p1} is drawn from a uniform distribution between 0 and 2π.

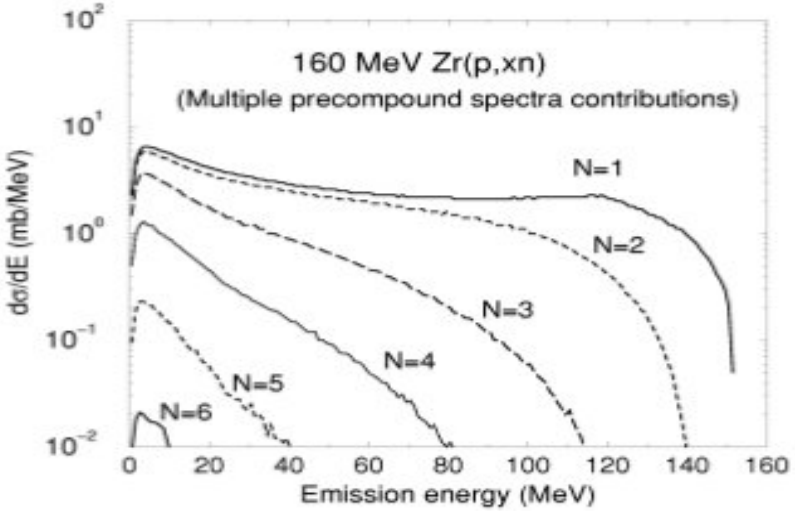
3) The momentum of the remaining particle is determined by momentum conservation.

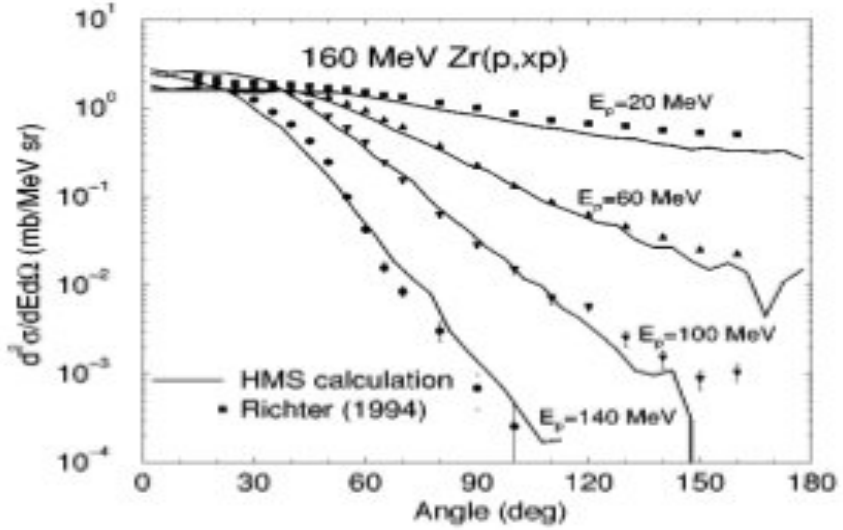
The energy of an emitted particle is corrected to take into account its binding energy, which is calculated exactly. Its angle of emission is assumed to remain the same as before emission.

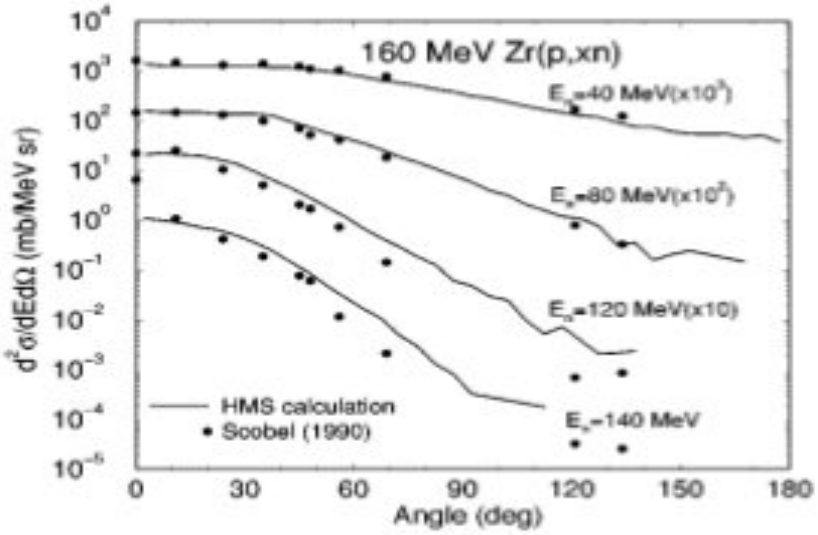
Recoil of the residual nucleus is also taken into account at each emission.

The double differential HMS – DDHMS - III

The DDHMS module in EMPIRE can perform calculations using densities of states of either equidistantly spaced single-particle levels or Fermi gas levels with linear momentum conservation.







From M. Blann, M. B. Chadwick, Phys. Rev. C **57** (1998) 233.

DDHMS – Kikuchi- Kawai - I

The exact linear momentum distributions for a particle scattering in a Fermi gas to create a 2p-1h state were determined by Kikuchi and Kawai. These distributions do not easily permit Monte Carlo selection of the particle and hole momenta.

However, in the frame in which

$$\vec{k}_{p0} = \frac{k_{p0}}{|\vec{k}_{p0} - \vec{k}_h|} \begin{pmatrix} -k_h \sin\theta_h \\ 0 \\ k_{p0} - k_h \cos\theta_h \end{pmatrix}$$

and

$$\vec{k}_h = -\frac{k_h}{|\vec{k}_{p0} - \vec{k}_h|} \begin{pmatrix} k_{p0} \sin\theta_h \\ 0 \\ k_h - k_{p0} \cos\theta_h \end{pmatrix}$$

so that

$$\vec{k}_{p0} - \vec{k}_h = \begin{pmatrix} 0 \\ 0 \\ |\vec{k}_{p0} - \vec{k}_h| \end{pmatrix}$$

K. Kikuchi, M. Kawai, *Nuclear Matter and Nuclear Reactions*, (North-Holland, Amsterdam,1968), p. 44.
D.F. Mega, B.V. Carlson, EPJ Web of Conferences **21** (2012) 09001.

DDHMS – Kikuchi- Kawai - II

One can write the final particle momenta as

$$\vec{k}_{p1} = \frac{k_{p1}}{|\vec{k}_{p1}+\vec{k}_{p2}|} U(\phi_{12}) \begin{pmatrix} -k_{p2}\sin\theta_{12} \\ 0 \\ k_{p1}+k_{p2}\cos\theta_{12} \end{pmatrix}$$

since then

$$\vec{k}_{p1}+\vec{k}_{p2} = \begin{pmatrix} 0 \\ 0 \\ |\vec{k}_{p1}+\vec{k}_{p2}| \end{pmatrix}$$

and

$$\vec{k}_{p2} = \frac{k_{p2}}{|\vec{k}_{p1}+\vec{k}_{p2}|} U(\phi_{12}) \begin{pmatrix} k_{p1}\sin\theta_{12} \\ 0 \\ k_{p2}+k_{p1}\cos\theta_{12} \end{pmatrix}$$

The particle/hole energies can be randomly drawn as before. The relative angle between the initial nucleon p0 and the hole can then be drawn from the distribution

$$P(\cos\theta_h) = \frac{2k_h}{\sqrt{k_{p0}^2 + k_h^2 - 2k_{p0}k_h\cos\theta_h}}$$

The angle θ_{12} is then determined by momentum conservation and the angle ϕ_{12} and a similar angle ϕ_h can be drawn from the interval 0 to 2π.

Summary

At low incident energy, nuclear reactions occur on two distinct time scales. Direct reactions, in which the incident particle remains in the continuum, occur quickly. Compound nucleus reactions, in which the projectile is trapped in a quasi-bound state, occur much more slowly.

Physically, the equilibration process proceeds through a series of nucleon-nucleon reactions. As the incident energy increases, it becomes more and more likely that one of the nucleons still retains a large fraction of the incident energy after the first one or two collisions, which favors its emission from a preequilibrium configuration

Semiclassical pre-equilibrium models describe the equilibration process through a series of incoherent nucleon-nucleon collisions and provide a reasonable description of particle emission except at low excitation energies and backwards angles, where coherent quantum effects can be important. We will discuss these in the next seminar.