Preequilibrium in Geant4

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12th Geant4 Collaboration Meeting, Hebden House,
September 17, 2007

Outline

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   - Cascade Exciton Model (CEM) , Gudima et al, 1983
   - Basic formulation
   - Work in progress ..

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- Geant4 version : simplistic *ad hoc* charged particle bookkeeping

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Basic assumption of preequilibrium models

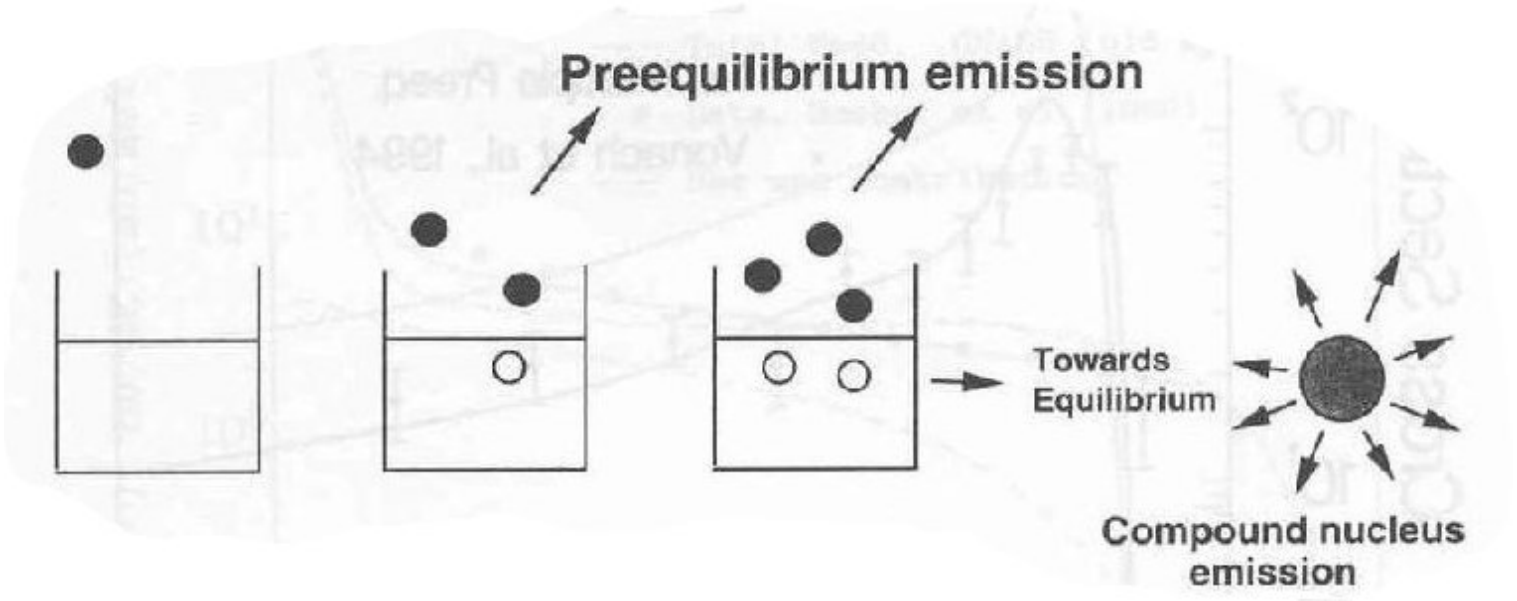

Figure: evolution towards equilibrium

The equillibration process proceeds through a series of nucleon-nucleon reactions.

The master equation

$$\frac{\partial P(E,n,t)}{\partial t} = -\Lambda(n,E)P(E,n,t) + \lambda_+(n-2,E)P(E,n-2,t) + \lambda_0(n,E)P(E,n,t) + \lambda_-(n+2,E)P(E,n+2,t) + \sum_j \int dT \int dE' \lambda_c^j(n+n_j,E',T)P(E',n+n_j,t)\delta(E'-E-B_j-T$$

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- The other ("less" important) trasition rates are obtained from it:

$$\lambda_0(p,h,E) = \frac{< \sigma(v_{rel} v_{rel} >}{V_{int}} \frac{n+1}{n} \left[\frac{gE - \mathcal{A}(p,h)}{gE - \mathcal{A}(p+1,h+1)}\right]^{n+1} \frac{p(p-1) + 4ph + h(h-1)}{gE - \mathcal{A}(p,h)}$$

The ingredients (II): particle emission rates

- The particle emission probability distribution:

$$\lambda_c^j(p,h,E,T) = \frac{2s_j+1}{\pi^2\hbar^3}\mu_j\mathcal{R}_j(p,h)\frac{\omega(p-1,h,E-B_j-T)}{\omega(p,h,E)}T\sigma_{inv}(T$$

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- The total emission rate:

$$\Gamma_j(p,h,E) = \int_{V_j^c}^{E-B_j}\lambda_j^c(p,h,E,T)dT$$

The ingredients (III): the total decay rate

$$\begin{aligned}\Lambda(p,h,E) &= \lambda_+(p,h,E)+\lambda_0(p,h,E)\\ &\quad +\lambda_-(p,h,E)+\sum_j \Gamma_j(p,h,E)\end{aligned}$$

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- $$\frac{d^2\lambda_n(\epsilon,\Omega)}{d\epsilon d\Omega} = \frac{2\mu\epsilon\sigma_{inv}}{\pi^2\hbar^3}\frac{\omega(p_r,h_r,E-\epsilon_\Omega,\vec{K}-\vec{k_\Omega})}{4\pi\omega(p,h,E,\vec{K})}$$

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- $$\sigma^2 = n_r\left(\frac{2m\epsilon_{av}}{3}\right)$$

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- *entrance channel memory concentrated here*:

$$a_n = \frac{3\sqrt{(\epsilon_{in} + B_{in} + \epsilon_F)(\epsilon + B_{em} + \epsilon_F)}}{n_r\epsilon_{av}\zeta}$$

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Soft *cutoff* criterium

- In *G4PreCompoundModel* class, the choice of preequilibrium transition/emission vs equilibrium transition is made with tis probability:

$$\begin{aligned} \textit{if} \quad n < n_{eq} \quad &\rightarrow \quad P_{pe}(n) = 1 - e^{-\frac{1}{0.32}(\frac{n}{n_{eq}}-1)^2} \\ \textit{if} \quad n \geq n_{eq} \quad &\rightarrow \quad P_{pe}(n) = 0 \end{aligned}$$

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- What is the impact of the preequilibrium to equilibrium transition sharpness on results?

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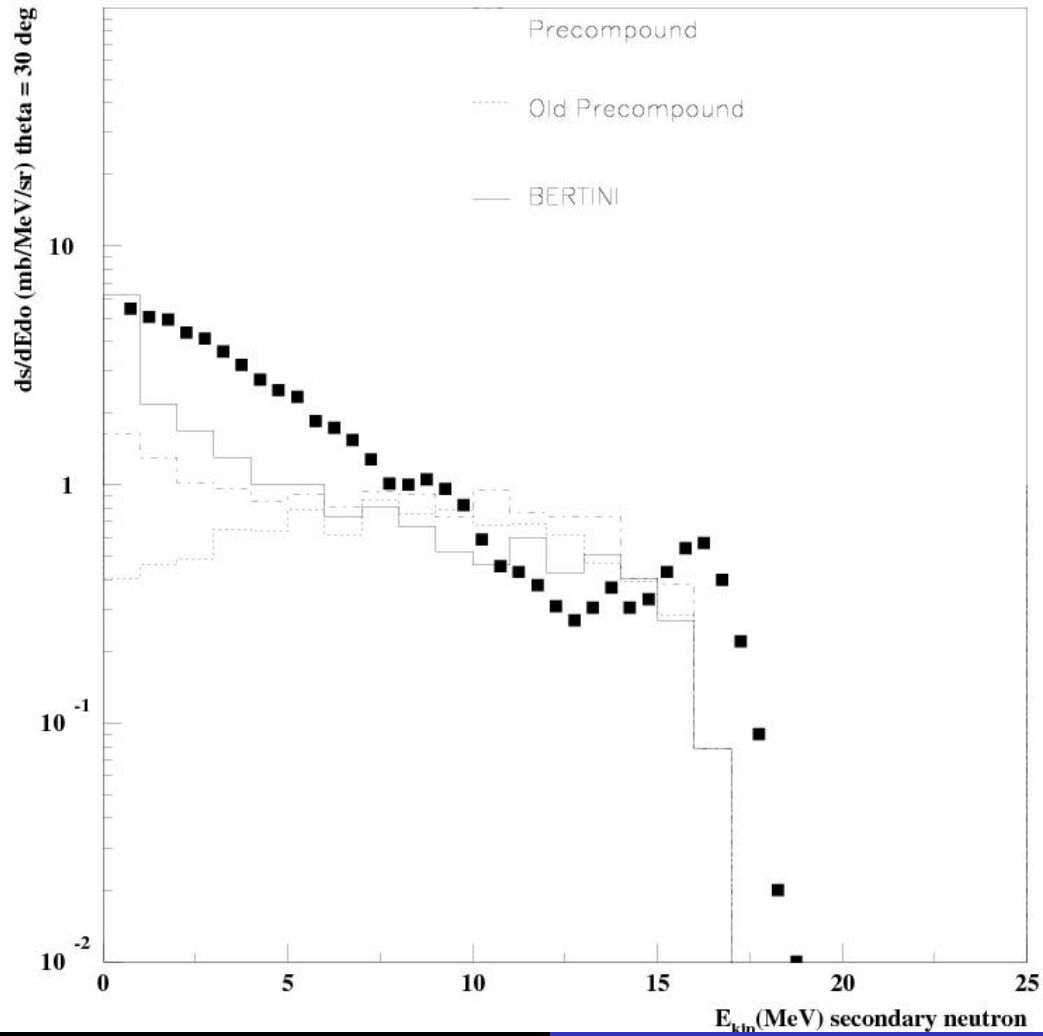
- G4EvaporationProbability:
  - Spurious *atomic mass factor* for cluster emission probability calculation (enhances it artificially and **greatly**)

Fixes (II)

In angular distribution calculation, incident direction must be transformed to CMS (**it was not**) in order to calculate emission angle θ_{CMS} by properly rotating from $\vec{k_\Omega}$ direction to z_{CMS} axis. Of course, Lorentz boost follows to transform to Lab system

Open question: test case $p + Al$ @ 22 MeV



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- Probably *refitting* of parameters (wrt one component situation) would be needed

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- Microscopic preformation factors $F_{l,m}$ (Sato, Iwamoto & Harada, 1983)
- Involved calculation of $F_{l,m}$, but parameterized and coded (together with Q_β) in *PCROSS* code for EM calculations.

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- *Still* a semiclassical method
- **DRAWBACK :** Cluster emission is not included

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- and similarly for an incident proton

$$P_{pp} = \frac{Z}{Z+3(A-Z)},$$

$$P_{pn} = 1 - P_{pp}.$$

Some hints of the formalism (II)

The energy distribution of the scattered particles $P(\varepsilon)$ is given by the ratio of the $(n-1)$ and n-exciton level densities ρ_n

$$P(\varepsilon)d\varepsilon = \frac{\rho_{n-1}(E-\varepsilon)g}{\rho_n(E)}d\varepsilon,$$

with $n = 2\,or\,3$ and

$$\rho_2(E) = \frac{g(gV)}{2} \;\; if \;\; E > V,$$

$$\rho_2(E) = \frac{g(gE)}{2} \;\; if \;\; E \leq V,$$

$$\rho_3(E) = \frac{g^3\left[V(2E-V)\right]}{4} \;\; if \;\; E \geq V.$$

where ε is the particle's energy above the Fermi energy and V is the potential well depth.

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The emission probability is calculated as

$$P_\nu(\varepsilon - B) = \frac{\lambda_c(\varepsilon - B)}{\lambda_c(\varepsilon - B) + \lambda_+(\varepsilon)},$$

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Outline

1. Present situation
   - Cascade Exciton Model (CEM) , Gudima et al, 1983
   - Basic formulation
   - Work in progress ..
2. Further development:
   - INCL+evaporation (Aatos)
   - Proposal 1: Improvements in Exciton Model (IEM)
   - Proposal 2: HMS (Hybrid MonteCarlo Sampling) model
3. For the future?:
   - Fully quantum mechanical models

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