UT-BATTELLE

HPC in Statistical Theories of Nuclear Reactions

SciDAC Workshop

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Pack Forest, WA

Physics:

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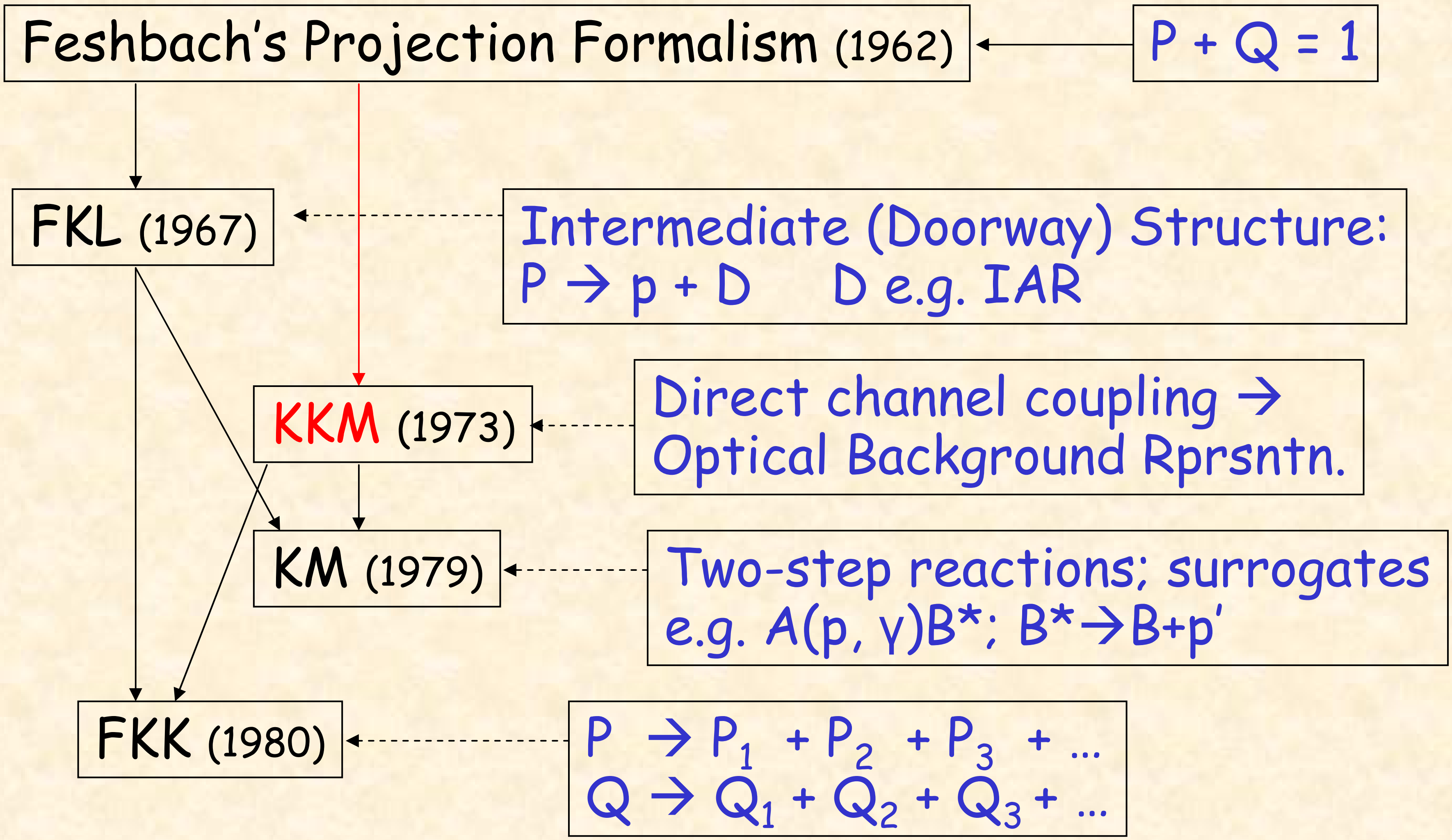
Overview

- KKM theory overview
- Numerical Tests of KKM central result on 1 CPU
- Parallelized eigensolver, matrix-multiplication, and disk I/O (Ken Roche) for numerical exploration of:
  - doorway state formalism
  - FKK theory of multistep pre-equilibrium reactions
  - Kerman-Sevgen theory, etc.


Feshbach's Projection Formalism (1962)
$P + Q = 1$
FKL (1967)
Intermediate (Doorway) Structure:
$P \rightarrow p + D$ D e.g. IAR
KKM (1973)
Direct channel coupling →
Optical Background Rprsntn.
KM (1979)
Two-step reactions; surrogates
e.g. A(p, γ)B*; B*→B+p′
FKK (1980)
$P \rightarrow P_1 + P_2 + P_3 + \ldots$
$Q \rightarrow Q_1 + Q_2 + Q_3 + \ldots$

Theory Summary

$$T_{cc'} = T_{cc'}^{(0)} + \frac{1}{2\pi}\sum_{\hat{q}} \frac{\hat{g}_{cq}\hat{g}_{c'q}}{E-\hat{\mathcal{E}}_q} \qquad \hat{g}_{cq} \equiv \sqrt{2\pi}\left\langle \chi_c^{(-)} \middle| H_{PQ} \middle| \hat{q} \right\rangle$$

KKM

$$T_{cc'} = T_{cc'}^{\text{opt}} + \frac{1}{2\pi}\sum_{q} \frac{g_{cq}g_{c'q}}{E-\mathcal{E}_q} \qquad g_{cq} \equiv \sqrt{2\pi}\left\langle \overline{\Psi}_c^{(-)} \middle| V_{PQ} \middle| q \right\rangle$$

$$\overline{\sigma_{cc'}^{\text{fl}}} \sim X_{cc}X_{c'c'} + X_{cc'}X_{c'c} \qquad X_{cc'} = \left\langle g_{cq}g_{c'q}^{*} \right\rangle_q$$

$$\overline{\sigma_{cc'}^{\text{fl}}} \sim \frac{1}{\sum P_{c''}}\left\{P_{cc}P_{c'c'} + P_{cc'}P_{cc'} + \ldots\right\} \qquad P_{cc'} = (1-\overline{S}\,\overline{S}^{*})_{cc'} = X_{cc'}Tr(X) + (X^2)_{cc'}$$

KM

$$\overline{\sigma_{Rc}^{\text{fl}}} \sim X_{RR}X_{cc} + X_{Rc}X_{cR} \qquad X_{Rc} = \left\langle \mathcal{M}_{Rq}g_{cq} \right\rangle_q$$

$$\mathcal{M}_{Rq} = M_R G_{\text{opt}} V_{Pq}$$

Projection operators

$$H\Psi = E\Psi$$

P – continuum space projection operator
Q – compound space projection operator

$$P + Q = 1 \;;\quad P \cdot Q = 0 \qquad P^2 = P \qquad H_{PQ} \equiv PHQ$$

$$(E - H_{PP})P\Psi = H_{PQ}Q\Psi$$

$$(E - H_{QQ})Q\Psi = H_{QP}P\Psi$$

$$(E - H_{PP})\chi = 0$$

$$\Rightarrow \quad P\Psi = \chi + \frac{1}{E - H_{PP}} H_{PQ}Q\Psi$$

$$\Rightarrow \quad T = T^{(0)} + \langle \chi | H_{PQ} | Q\Psi \rangle$$

$$(E - H_{QQ} - H_{QP}\frac{1}{E - H_{PP}}H_{PQ})Q\Psi = H_{QP}\chi$$

$$\Rightarrow \quad T = T^{(0)} + \left\langle \chi \middle| H_{PQ} \frac{1}{E - H_{QQ} - H_{QP}\frac{1}{E - H_{PP}}H_{PQ}} H_{QP} \middle| \chi \right\rangle$$

Projection operators cont'd.

$$T = T^{(0)} + \left\langle \chi \middle| H_{PQ} \frac{1}{E - H_{QQ} - H_{QP} G_P H_{PQ}} H_{QP} \middle| \chi \right\rangle$$

$$\left[H_{QQ} + H_{QP} G_P H_{PQ} \right] \left| \hat{q} \right\rangle = \hat{\mathcal{E}}_q \left| \hat{q} \right\rangle$$

$$\left\langle \tilde{\hat{q}} \right| \left[H_{QQ} + H_{QP} G_P H_{PQ} \right] = \left\langle \tilde{\hat{q}} \right| \hat{\mathcal{E}}_q$$

$$\hat{\mathcal{E}}_q = \hat{E}_q - i \frac{\hat{\Gamma}_q}{2}$$

$$\sum_{\hat{q}} \left| \hat{q} \right\rangle \left\langle \tilde{\hat{q}} \right| = 1$$

$$\left\langle \tilde{\hat{q}} \middle| \hat{q}' \right\rangle = \delta_{\hat{q}\hat{q}'}$$

$$H_{QQ} \left| Q_j \right\rangle = E_{Q_j} \left| Q_j \right\rangle$$

$$\sum_j \left| Q_j \right\rangle \left\langle Q_j \right| = 1$$

$$\left\langle Q_j \middle| Q_j \right\rangle = \delta_{ij}$$

$$T_{cc'} = T_{cc'}^{(0)} + \sum_{\hat{q}} \left\langle \chi_c \middle| H_{PQ} \middle| \hat{q} \right\rangle \frac{1}{E - \hat{\mathcal{E}}_q} \left\langle \tilde{\hat{q}} \middle| H_{QP} \middle| \chi_{c'} \right\rangle$$

$$T_{cc'} = T_{cc'}^{(0)} + \frac{1}{2\pi} \sum_{\hat{q}} \frac{\hat{g}_{cq} \hat{g}_{c'q}}{E - \hat{\mathcal{E}}_q}$$

KKM:

Two-potential formula:

Kawai, Kerman, and McVoy
Ann. of Phys. 75, 156 (1973)

$$T = T^{\mathrm{opt}} + \left\langle \overline{P\Psi} \right| V_{PQ} \frac{1}{E - H_{QQ} - V_{QP} G_{\mathrm{opt}} V_{PQ}} V_{QP} \left| \overline{P\Psi} \right\rangle$$

$$\left[H_{QQ} + V_{QP} G_{\mathrm{opt}} V_{PQ} \right] \left| q \right\rangle = \mathcal{E}_q \left| q \right\rangle$$

$$\left\langle \tilde{q} \right| \left[H_{QQ} + V_{QP} G_{\mathrm{opt}} V_{PQ} \right] = \left\langle \tilde{q} \right| \mathcal{E}_q$$

$$\mathcal{E}_q = E_q + i \frac{\Gamma_q}{2}$$

$$\sum_{\hat{q}} \left| q \right\rangle \left\langle \tilde{q} \right| = 1$$

$$\left\langle \tilde{q} \middle| q' \right\rangle = \delta_{qq'}$$

$$\left| q \right\rangle = \sum_j \left\langle Q_j \middle| q \right\rangle \left| Q_j \right\rangle$$

$$H_{QQ} \left| Q_j \right\rangle = E_{Q_j} \left| Q_j \right\rangle$$

$$\sum_j \left| Q_j \right\rangle \left\langle Q_j \right| = 1$$

$$\left\langle Q_j \middle| Q_j \right\rangle = \delta_{ij}$$

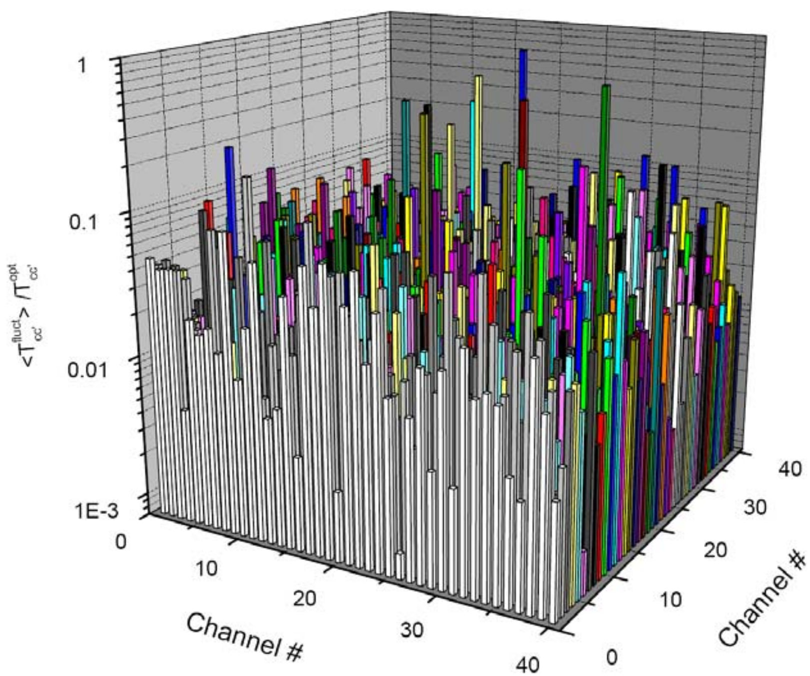
$$T_{cc'} = T_{cc'}^{\mathrm{opt}} + \sum_q \left\langle \overline{P\Psi_c} \right| V_{PQ} \left| \hat{q} \right\rangle \frac{1}{E - \mathcal{E}_q} \left\langle \tilde{\hat{q}} \right| V_{QP} \left| \overline{P\Psi}_{c'} \right\rangle$$

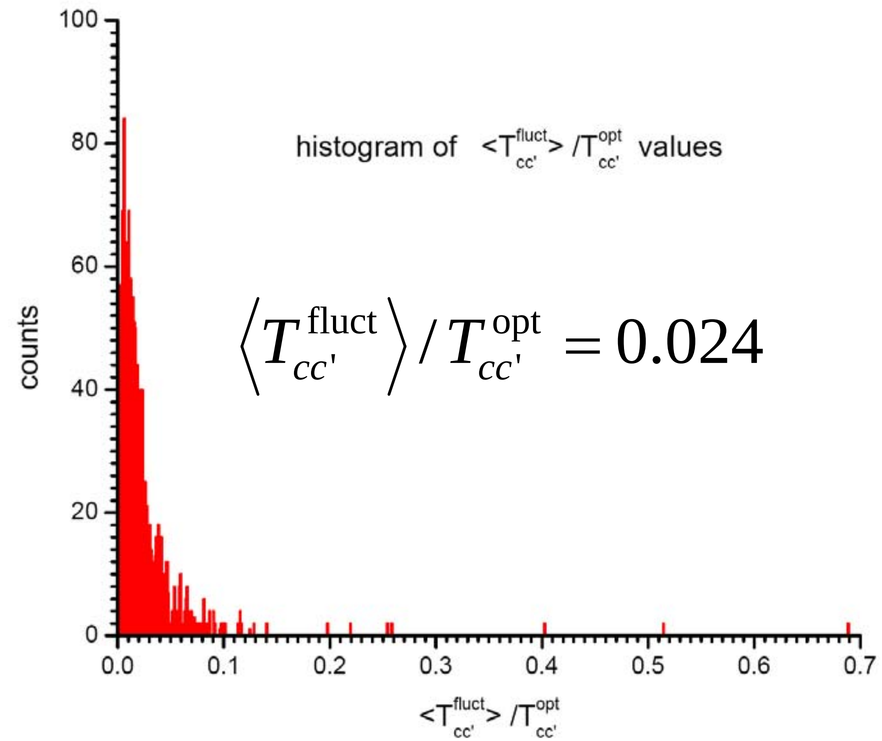
$$V_{PQ} = H_{PQ} \sqrt{\frac{iI}{E - H_{QQ} + iI}}$$

$$T_{cc'} = T_{cc'}^{\mathrm{opt}} + T_{cc'}^{\mathrm{fluct}} \quad , \quad T_{cc'}^{\mathrm{fluct}} \equiv \frac{1}{2\pi} \sum_q \frac{g_{cq} g_{c'q}}{E - \mathcal{E}_q} \Rightarrow \left\langle T_{cc'}^{\mathrm{fluct}} \right\rangle << T_{cc'}^{\mathrm{opt}} \quad \text{because} \quad \left\langle T_{cc'} \right\rangle \cong T_{cc'}^{\mathrm{opt}}$$

Verify numerically for
Gaussian random coupling H_{PQ}.

Numerical Test of $\langle T_{cc'}^{\text{fluct}} \rangle / T_{cc'}^{\text{opt}} << 1$





$$\langle T_{cc'}^{\text{fluct}} \rangle / T_{cc'}^{\text{opt}} = 0.024$$

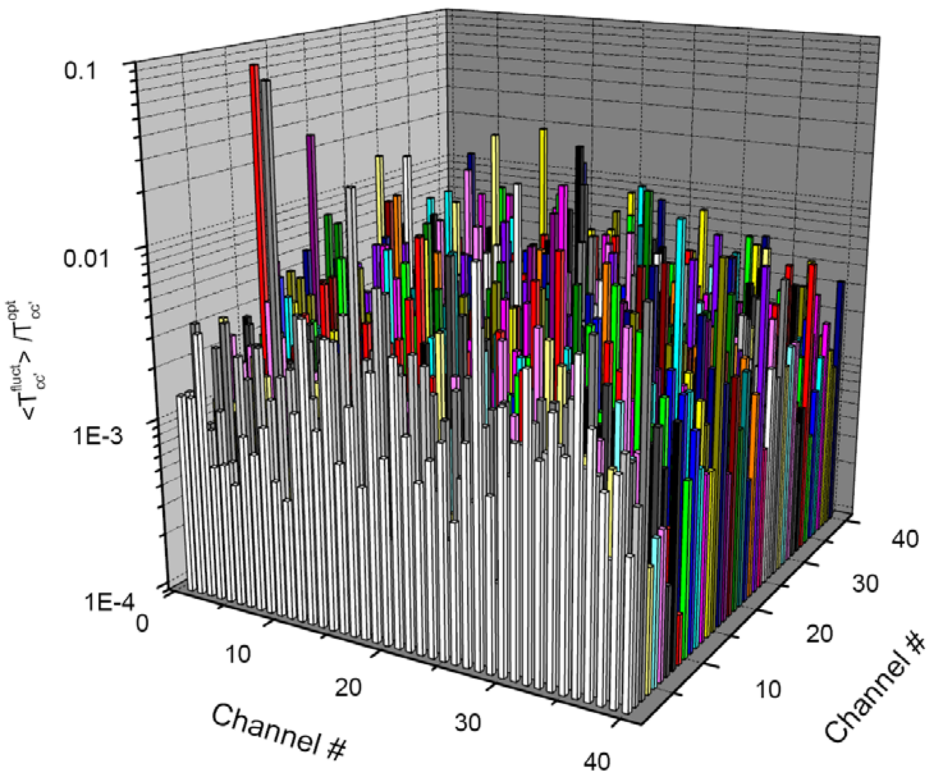
In the spirit of:
Dagdeviren and Kerman,
Ann. of Phys. **163** (1985) 199

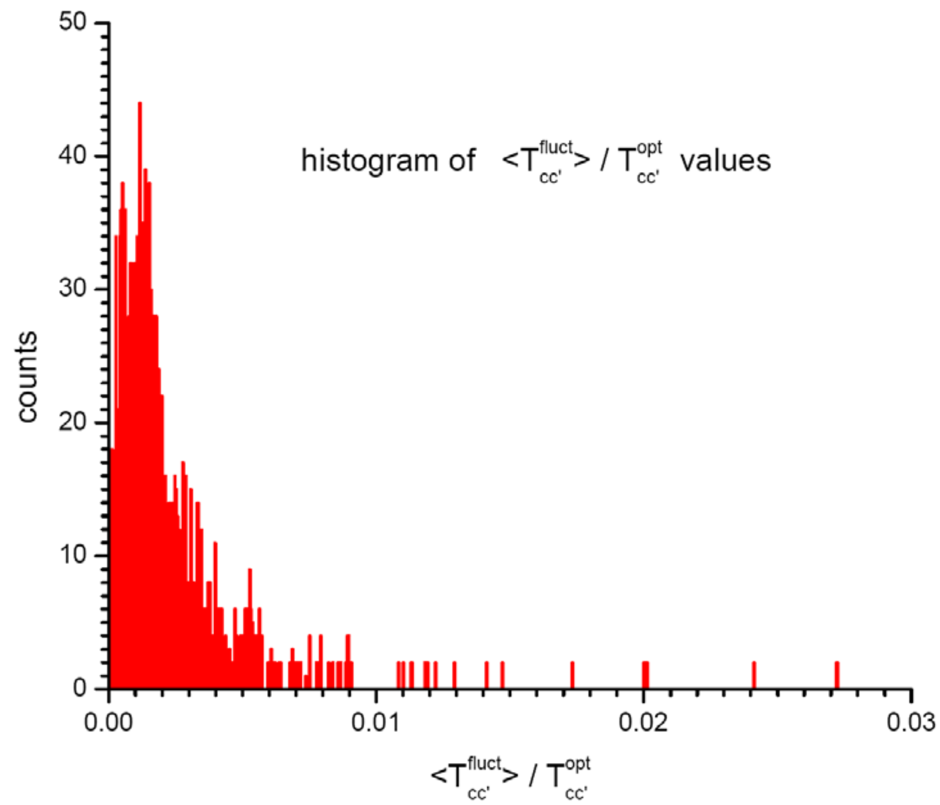
Computation parameters:

- 400 equidistant Q-levels
- 40 channels
- 20 equidistant radial points where H_{PQ} set to a Gaussian-distributed random interaction
- E = 20 MeV
- 100 E′ points for Lorentzian averaging between 18 and 22 MeV
- I = 0.5 MeV
- s-wave only
- $\Gamma/D >> 1$

Cont'd. (1,600 Q-levels)

$$\left\langle \left\langle T_{cc'}^{\text{fluct}} \right\rangle / T_{cc'}^{\text{opt}} \right\rangle = 0.0024$$





Approximations in KKM Cross-section

$$T_{cc'} = T_{cc'}^{\text{opt}} + \frac{1}{2\pi}\sum_q \frac{g_{qc}g_{qc'}}{E-\mathcal{E}_q}$$

$$\Rightarrow \left\langle \sigma_{cc'}^{\text{fl}} \right\rangle \sim \left\langle \left| T_{cc'} - \overline{T}_{cc'} \right|^2 \right\rangle_I \sim \left\langle \sum_{qq'} \frac{g_{qc}g_{qc'}}{E-\mathcal{E}_q} \frac{g_{q'c}^{*}g_{q'c'}^{*}}{E-\mathcal{E}_{q'}^{*}} \right\rangle_I$$

Random Phase Hypothesis
→ only q=q' contributes

$$\cong \left\langle \sum_q \frac{g_{qc}g_{qc'}}{E-\mathcal{E}_q} \frac{g_{qc}^{*}g_{qc'}^{*}}{E-\mathcal{E}_{q'}^{*}} \right\rangle_I$$

$$\cong 2\pi \left\langle \frac{g_{qc}g_{qc'}g_{qc}^{*}g_{qc'}^{*}}{D_q\Gamma_q} \right\rangle_{q(I)}$$

$$\cong \frac{2\pi}{D_q\Gamma_q} \left\langle g_{qc}g_{qc'}g_{qc}^{*}g_{qc'}^{*} \right\rangle_{q(I)}$$

$$\cong X_{cc}X_{c'c'} + X_{cc'}X_{c'c} \qquad \text{where} \qquad X_{cc'} \equiv \left(\frac{2\pi}{D\Gamma}\right)^{1/2} \left\langle g_{qc}g_{qc'}^{*} \right\rangle_{q(I)}$$

Effect of KKM approximations could be studied numerically

See Appendix in KKM for details

Conclusions and Outlook

- Year 2:
  - Single CPU program written (C. Bertulani & G. Arbanas)
  - Central result of KKM tested (CNR*07 AIP Proceedings)
- Year 3:
  - Parallelize the code (Ken Roche)
  - Tests of ALL approximations in KKM
  - Would like eigenvalues of matrix size of 10^6 x 10^6
  - Extend to Doorway reactions,
- Year 4-5
  - Extend the model to FKK multistep pre-equilibrium,
  - Kerman-Sevgen theory (cross-section covariance)
  - Study connections to RMT and Max. Entropy methods

KKM: Enhancement factor (σ/σ_{HF}) of KKM and Moldauer

(from Kawano, Bonneau, and Kerman, NDST 2007)

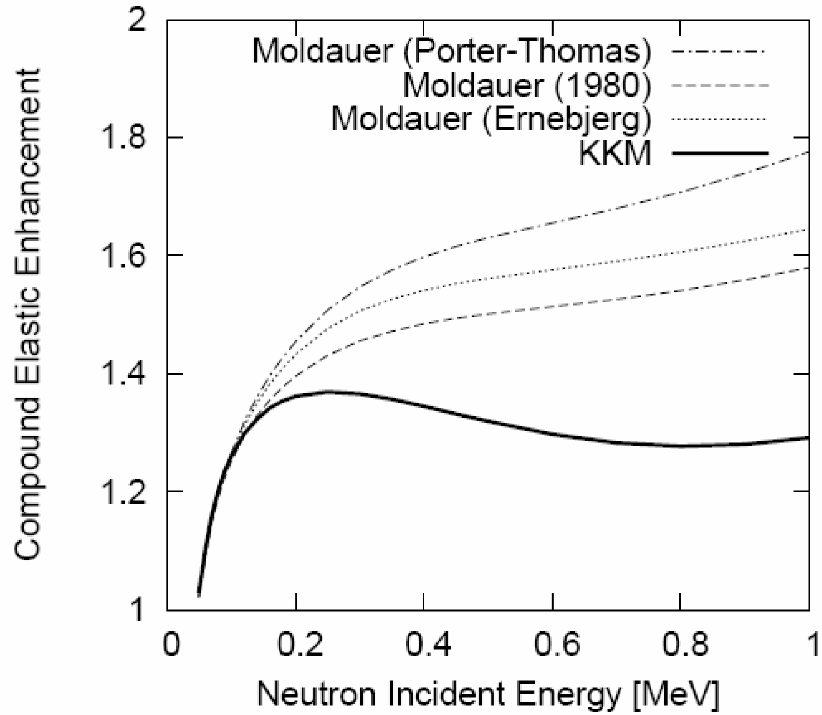


Fig. 2. Calculated compound elastic enhancement factors. The thick solid line is the KKM result, and the other lines are for the Moldauer calculations.

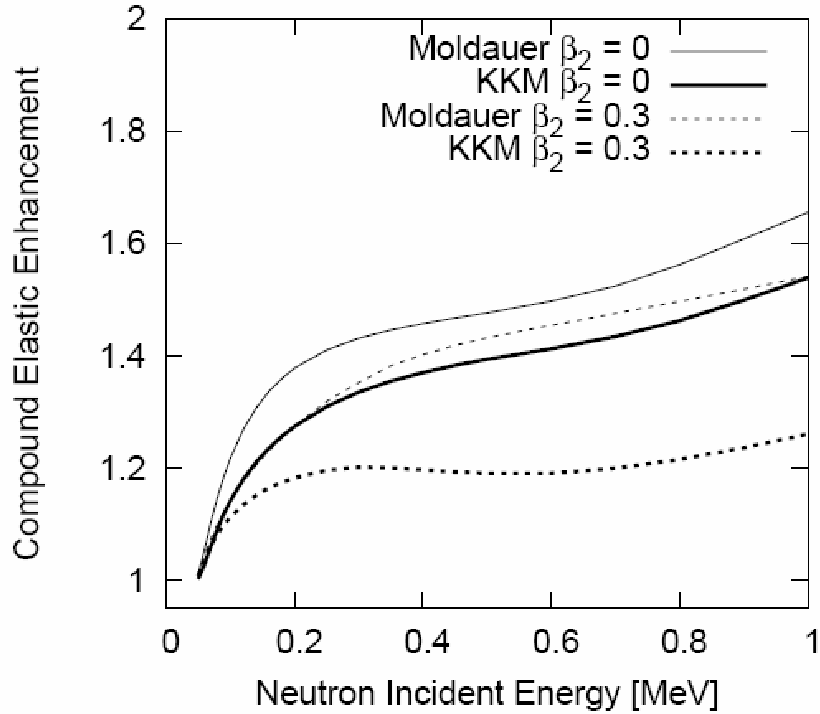


Fig. 3. Compound elastic enhancement factors for the spherical and strongly deformed cases. The thick lines are the KKM results, and the thin lines are for the Moldauer calculations.

CC on ^{238}U(n,n') ground state rotational band $0^+,2^+,4^+,6^+,8^+$

→ S-matrix → Transmission coefficients → X-matrix → σ_{KKM} vs. $\sigma_{cc'} = \frac{T_c T_{c'}}{\sum_a T_a} W_{cc'}$

The difference in U-238 total elastic cross-section is ~4%

KM T-matrix

$$T_{\rm Rc} = \left\langle \chi_{\rm i}^{(-)} \middle| M \middle| \chi_{\rm f}^{(+)} \Psi_c^{(+)} \right\rangle = M_R P\Psi_c^{(+)}$$

R=(i,f)

For example:
i - deuteron
f - proton
c - neutron

$$P\Psi_c = \overline{P\Psi}_c + G_{\rm opt} V_{PQ} \frac{1}{E - H_{QQ} - V_{QP} G_{\rm opt} V_{PQ}} V_{QP} \overline{P\Psi}_c$$

$$= \overline{P\Psi}_c + \sum_q G_{\rm opt} V_{Pq} \frac{1}{E - \mathcal{E}_q} V_{qP} \overline{P\Psi}_c$$

$$\Rightarrow \quad T_{\rm Rc} = T_{Rc}^{\rm opt} + \sum_q \frac{(M_R G_{\rm opt} V_{Pq}) g_{qc}}{E - \mathcal{E}_q}$$

$$= T_{Rc}^{\rm opt} + \sum_q \frac{\mathcal{M}_{Rq} g_{qc}}{E - \mathcal{E}_q}$$

$$= T_{Rc}^{\rm opt} + T_{Rc}^{\rm fluct}$$

KM fluctuation Cross-section

$$\left\langle \sigma_{Rc}^{\mathrm{fl}} \right\rangle \sim \left\langle \sum_{qq'} \frac{\mathcal{M}_{Rq} g_{qc}}{E - \mathcal{E}_q} \frac{\mathcal{M}_{Rq'}^{*} g_{q'c}^{*}}{E - \mathcal{E}_{q'}^{*}} \right\rangle_I$$

Random Phase Hypothesis

$$\cong \left\langle \sum_{q} \frac{\mathcal{M}_{Rq} g_{qc} \mathcal{M}_{Rq}^{*} g_{qc}^{*}}{(E - \mathcal{E}_q)(E - \mathcal{E}_q^{*})} \right\rangle_I$$

Analogous to KKM

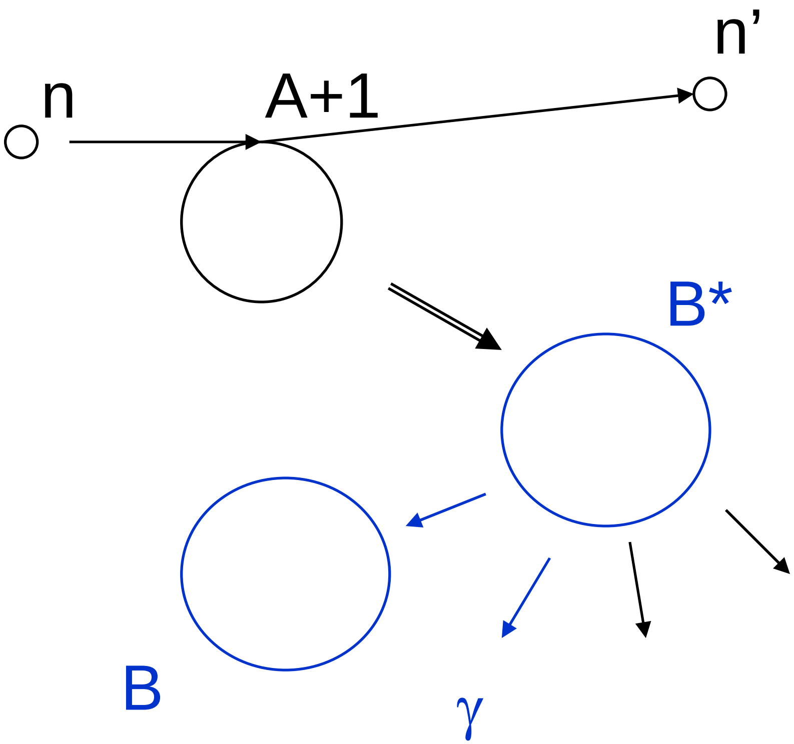
$$\cong 2\pi \left\langle \frac{\mathcal{M}_{Rq} g_{qc} \mathcal{M}_{Rq}^{*} g_{qc}^{*}}{D_q \Gamma_q} \right\rangle_{q(I)}$$

$$\cong \frac{2\pi}{D_q \Gamma_q} \left\langle \mathcal{M}_{Rq} g_{qc} \mathcal{M}_{Rq}^{*} g_{qc}^{*} \right\rangle_{q(I)}$$

$$\cong X_{RR} X_{cc} + X_{Rc} X_{cR} \qquad X_{RR} = \left\langle \mathcal{M}_{Rq} \mathcal{M}_{Rq}^{*} \right\rangle_{q(I)} \qquad X_{Rc} = \left\langle \mathcal{M}_{Rq} g_{qc}^{*} \right\rangle_{q(I)}$$

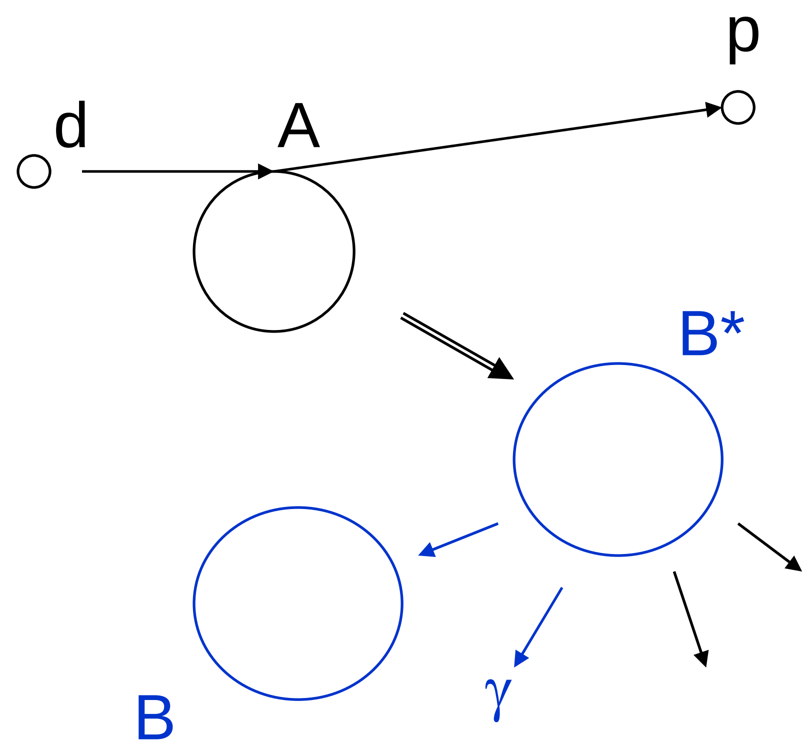
KM applied to Surrogate Reactions

"Desired" reaction, e.g. (n,n'γ)



$$\left\langle \sigma^{\mathrm{fl}}_{R'c} \right\rangle \cong X_{R'R'} X_{cc} + X_{R'c} X_{cR'}$$

Surrogate reaction, e.g. (d,pγ)



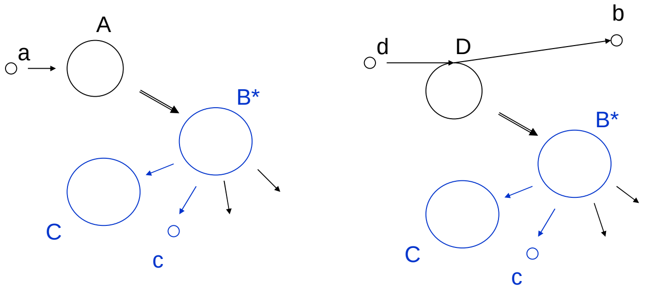
$$\left\langle \sigma^{\mathrm{fl}}_{Rc} \right\rangle \cong X_{RR} X_{cc} + X_{Rc} X_{cR}$$

Surrogate Reactions cont'd.

Desired reaction cross-section:

$$\frac{d\sigma_{\alpha\gamma}^{\mathrm{HF}}(E_\alpha)}{dE_\chi} = \sum_{J\pi} \sigma_\alpha^{\mathrm{CN}}(E_{\mathrm{ex}}, J, \pi)\, G_\chi^{\mathrm{CN}}(E_{\mathrm{ex}}, J, \pi)\;\; W$$

$$\alpha = (a + A)$$
$$\chi = (c + C)$$
$$\delta = (d + D)$$
$$E_{\mathrm{ex}} = S_a(B) + E_\alpha$$
$$= S_c(B) + E_\chi$$



Surrogate reaction probability:

$$P_{\delta\gamma}(E_{\mathrm{Ex}}) = \sum_{J\pi} F_\delta(E_{\mathrm{ex}}, J, \pi)\, G_\chi^{\mathrm{CN}}(E_{\mathrm{ex}}, J, \pi)$$

Jπ distributions are likely different for the two reactions:
complicates calculations and requires more surrogate data

J. Escher, F. Dietrich,
Phys. Rev. C74, 054601 (2006)

KKM

Kawai, Kerman, and McVoy
Ann. of Phys. 75, 156 (1973)

$$(E - H_{PP})P\Psi = H_{PQ}\Psi \qquad (1)$$

$$(E - H_{QQ})Q\Psi = H_{QP}\Psi \qquad (2)$$

$$Q\Psi = \frac{1}{E - H_{QQ}} H_{QP}\Psi$$

$$(E - H_{PP} - H_{PQ}\frac{1}{E - H_{QQ}} H_{QP})P\Psi = 0 \qquad (3)$$

Lorentz. average, width I

$$(E - H_{PP} - H_{PQ}\frac{1}{E - H_{QQ} + iI} H_{QP})\overline{P\Psi} = 0$$

$$(E - H_{\text{opt}})\overline{P\Psi} = 0$$

Subtract H_{opt} from both Sides of (3)

$$(E - H_{opt})P\Psi = H_{PQ}\left(\frac{1}{E - H_{QQ}} - \frac{1}{E - H_{QQ} + iI}\right)H_{QP}\Psi$$

$$= V_{PQ}G_Q V_{QP} P\Psi$$

Two-pot. V_1, V_2

$$V_{PQ} \equiv H_{PQ}\sqrt{\frac{iI}{E - H_{QQ} + iI}}$$

$$\left(\frac{1}{E - H_{QQ}} - \frac{1}{E - H_{QQ} + iI}\right) = \frac{iI}{(E - H_{QQ})(E - H_{QQ} + iI)}$$

$$= \sqrt{\frac{iI}{E - H_{QQ} + iI}}\,\frac{1}{E - H_{QQ}}\,\sqrt{\frac{iI}{E - H_{QQ} + iI}}$$

KKM cont'd.

Separation of w.f. into average and fluctuating parts:

(also used in KM)

Used identities:
$(1-x)^{-1} = 1+x+x^2+\ldots$
$(AB)^{-1}=B^{-1}A^{-1}$
$X(1-YX)^{-1}=(1-XY)^{-1}X$

$$(E-H_{opt})P\Psi = V_{PQ}G_Q V_{QP}\Psi$$

$$\begin{aligned}
\Rightarrow \quad P\Psi &= \overline{P\Psi} + G_{\text{opt}}V_{PQ}G_Q V_{QP}\Psi \\
&= \overline{P\Psi} + G_{\text{opt}}V_{PQ}G_Q V_{QP}\left[1 + G_{\text{opt}}V_{PQ}G_Q V_{QP} + \ldots\right]\overline{P\Psi} \\
&= \overline{P\Psi} + G_{\text{opt}}V_{PQ}G_Q V_{QP}\frac{1}{1-G_{\text{opt}}V_{PQ}G_Q V_{QP}}\overline{P\Psi} \\
&= \overline{P\Psi} + G_{\text{opt}}V_{PQ}G_Q\frac{1}{1-V_{QP}G_{\text{opt}}V_{PQ}G_Q}V_{QP}\overline{P\Psi} \\
&= \overline{P\Psi} + G_{\text{opt}}V_{PQ}\frac{1}{E-H_{QQ}-V_{QP}G_{\text{opt}}V_{PQ}}V_{QP}\overline{P\Psi}
\end{aligned}$$