Averaging Over Resonances

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Outline

- **Overview: Kawai-Kerman-McVoy (KKM) statistical theory of nuclear reactions**
- **Numerical verification of KKM results**
- **Extension of KKM to Doorways**
- **Accomplishments, the remaining tasks, and plans for the next year**

Energy structures in cross sections

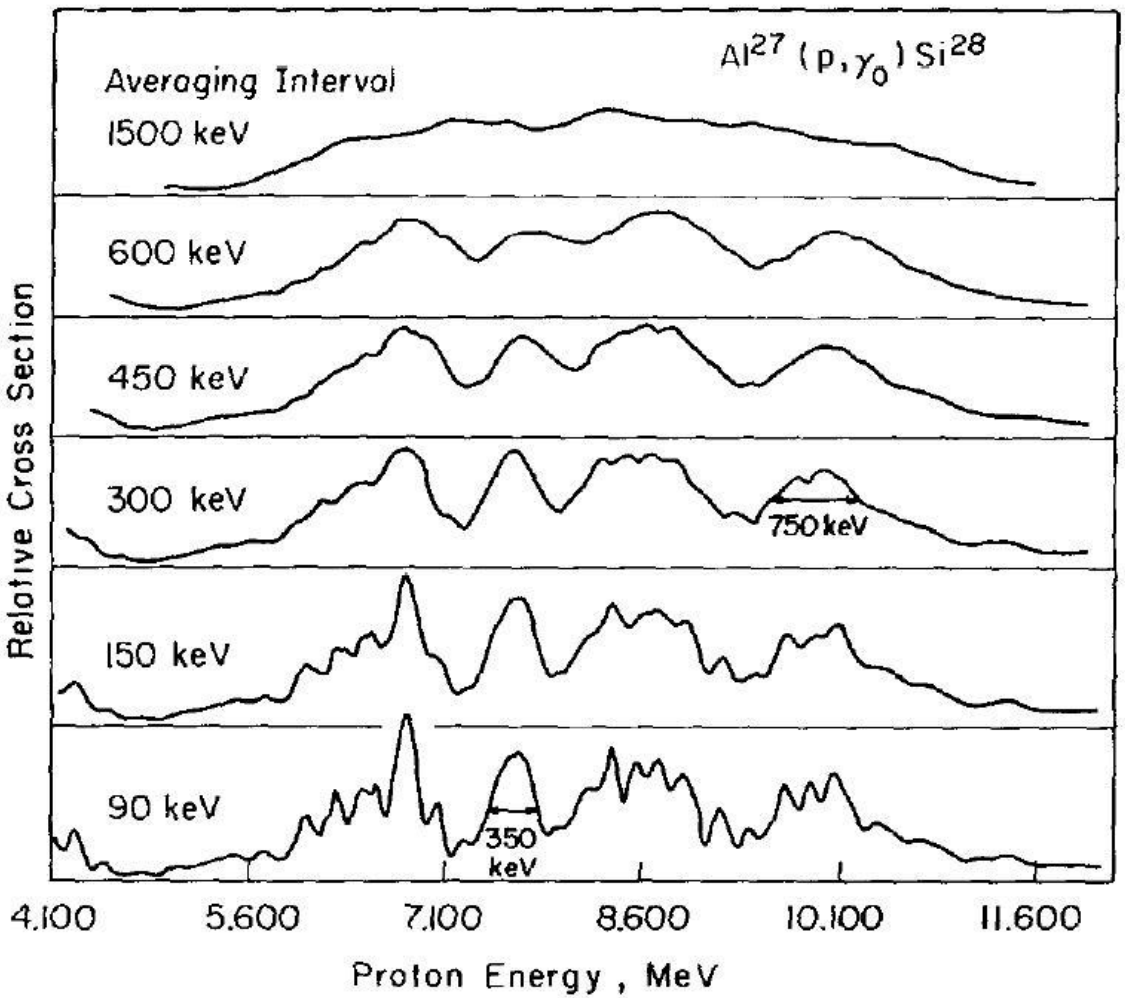
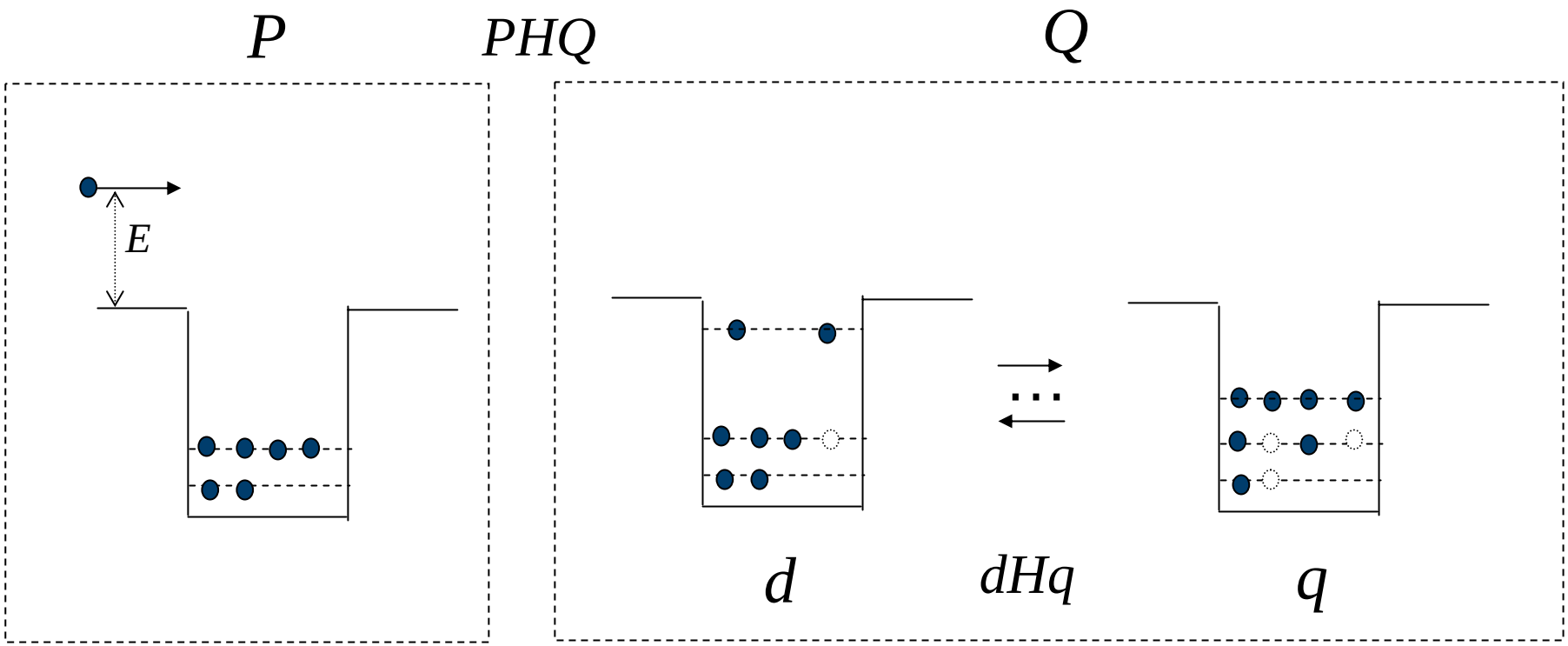
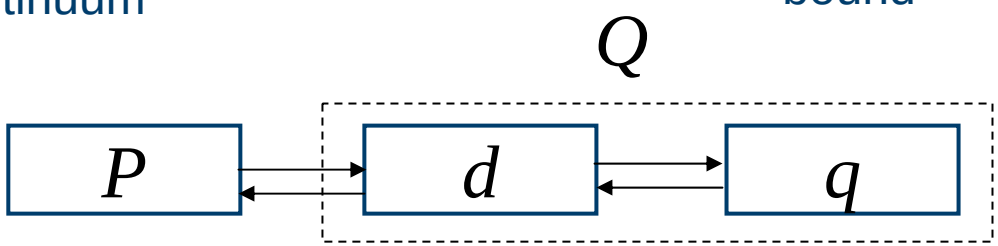


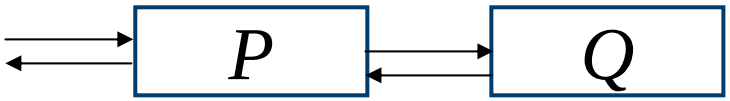
FIG. 6. Photocapture of protons by Al^{27} to the ground state of Si^{28}. The data is presented for various stages of resolution. From ref. *26*.

Physical picture





KKM Introduction



Projection operators:

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

$$H\Psi = E\Psi$$

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

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

Two-potential formula: H_{PP}, H_{PQ}

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

$$\Rightarrow \qquad T = T^{\mathrm{dir}} + \left\langle \chi \middle| H_{PQ} \frac{1}{E-H_{QQ}-H_{QP}\dfrac{1}{E-H_{PP}}H_{PQ}} H_{QP} \middle| \chi \right\rangle$$

$$T = T^{\mathrm{dir}} + T^{\mathrm{res}} \Rightarrow \langle T^{\mathrm{res}} \rangle_I \neq 0$$

➔Cross terms in cross section: $\langle \sigma \rangle_I \sim \langle |T|^2 \rangle_I$

KKM Introduction

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

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

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

$$\hat{\varepsilon}_q = \hat{E}_q - i \frac{\hat{\Gamma}_q}{2} \qquad H_{QQ} \left| Q_j \right\rangle = E_{Q_j} \left| Q_j \right\rangle$$

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

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

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

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

Matrix size limited by the eigensolver:
1 CPU < 10^4,
in parallel < 10^6

KKM Summary

- **KKM Two-pot. T-matrix:**
  - **Optical ("opt"),** H^{opt}
  - **Fluctuating ("fl"),** V_{PQ}

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

$$\boxed{\begin{aligned}(E - H_{PP}^{\text{opt}})P\Psi &= V_{PQ}Q\Psi \\ (E - H_{QQ})Q\Psi &= V_{QP}P\Psi\end{aligned}}$$

Two-potential formula: H^{opt}, $V_{PQ}(H_{PQ},I)$

$$(E - H_{PP}^{\text{opt}})\Psi^{\text{opt}} = 0$$

$$\Rightarrow \quad T = T^{\text{opt}} + \left\langle \Psi^{\text{opt}} \middle| V_{PQ} \frac{1}{E - H_{QQ} - V_{QP}\dfrac{1}{E - H_{PP}^{\text{opt}}}V_{PQ}} V_{QP} \middle| \Psi^{\text{opt}} \right\rangle$$

$$T = T^{\text{opt}} + T^{\text{fluct}}$$

$$T^{\text{opt}} = \langle T \rangle_I \Rightarrow \langle T^{\text{fluct}} \rangle_I \approx 0$$

This simplifies cross section: $\langle \sigma \rangle_I \sim \langle |T|^2 \rangle_I$

KKM Summary

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

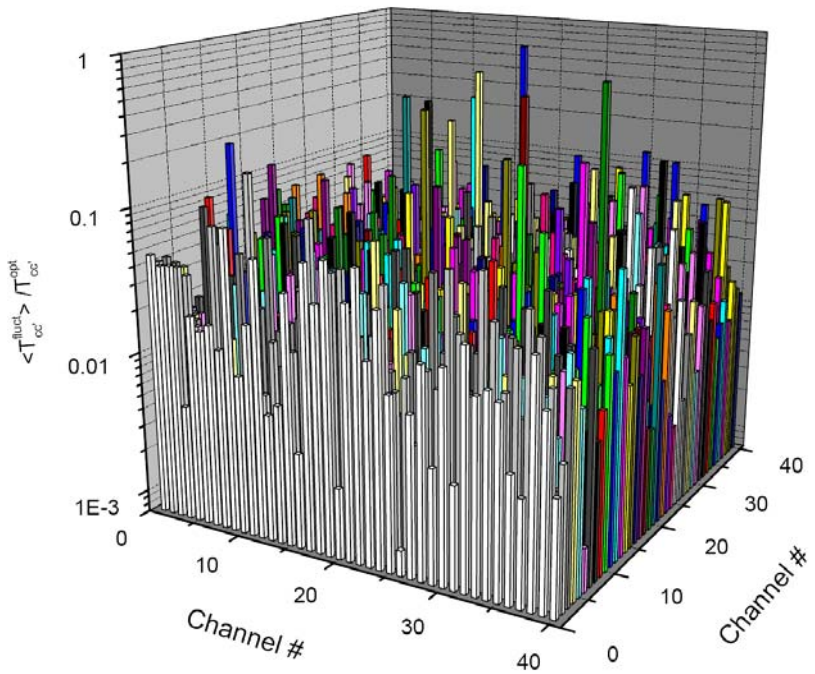
- **Two-potential T-matrix:**
  - **Direct ("P")**
  - **Resonant ("Q")**
- **KKM Two-pot. T-matrix:**
  - **Optical ("opt")**
  - **Fluctuating ("fl")**

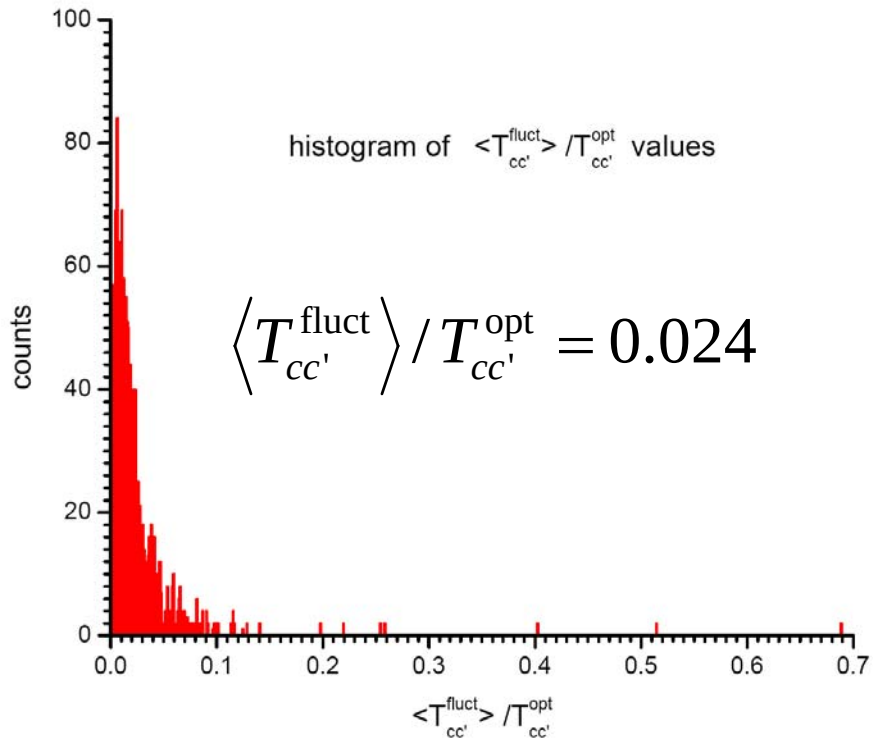
$$T_{cc'} = T_{cc'}^{\mathrm{dir}} + T_{cc'}^{\mathrm{res}} \quad , \quad T_{cc'}^{\mathrm{dir}} \equiv \left\langle \phi_c \left| V_{PP} \right| \Psi_{c'} \right\rangle, \qquad T_{cc'}^{\mathrm{res}} \equiv \frac{1}{2\pi} \sum_q \frac{\hat{g}_{cq} \hat{g}_{c'q}}{E - \hat{\varepsilon}_q}$$

$$T_{cc'} = T_{cc'}^{\mathrm{opt}} + T_{cc'}^{\mathrm{fluct}} \quad , \quad T_{cc'}^{\mathrm{opt}} \equiv \left\langle \phi_c \left| V^{\mathrm{opt}} \right| \Psi^{\mathrm{opt}}{}_{c'} \right\rangle, \qquad T_{cc'}^{\mathrm{fluct}} \equiv \frac{1}{2\pi} \sum_q \frac{g_{cq} g_{c'q}}{E - \varepsilon_q}$$

$$\langle T_{cc'}^{\mathrm{fluct}} \rangle_I \approx 0$$

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





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

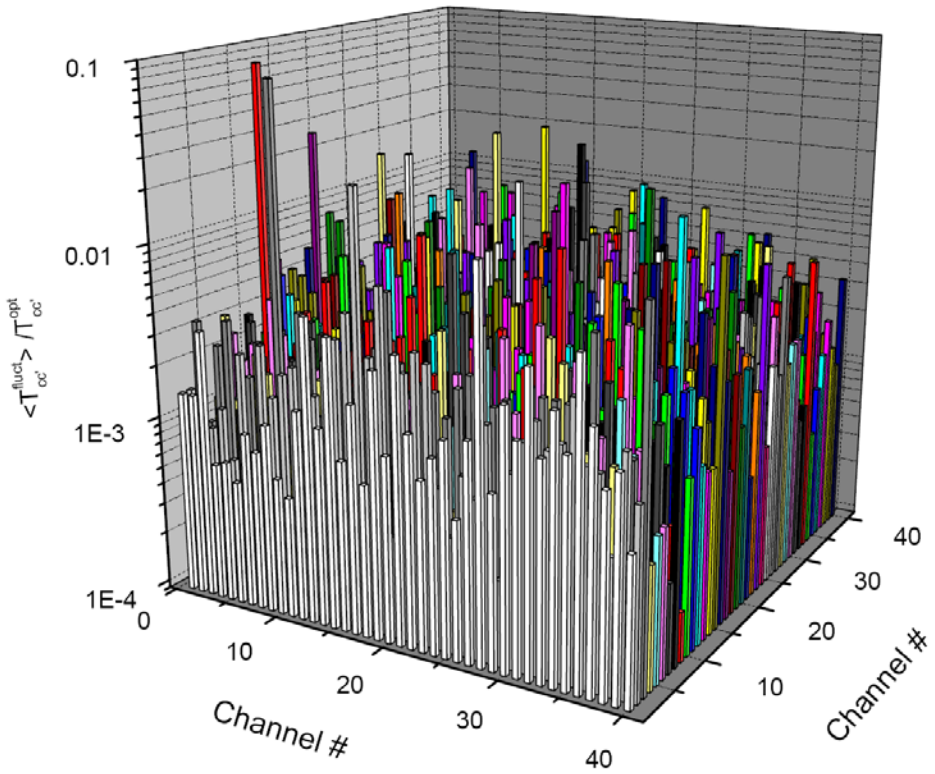
In the spirit of:
Dagdeviren and Kerman,
Ann. of Phys. **163** (1985) 199

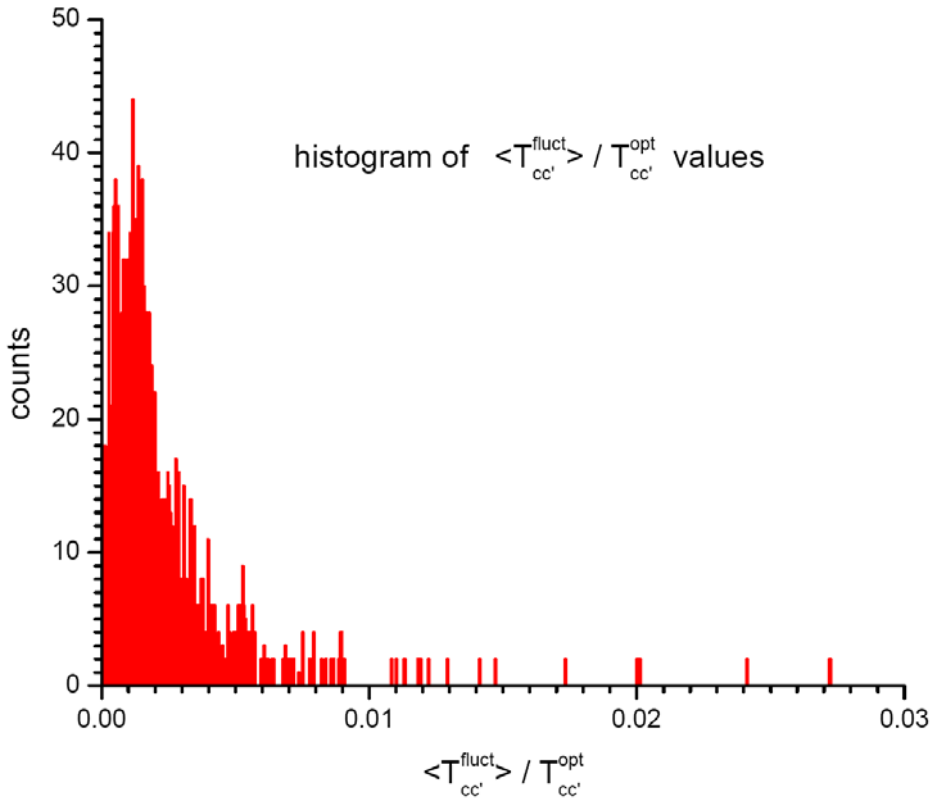
Computation parameters:

- 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
- $\Gamma/D >> 1$

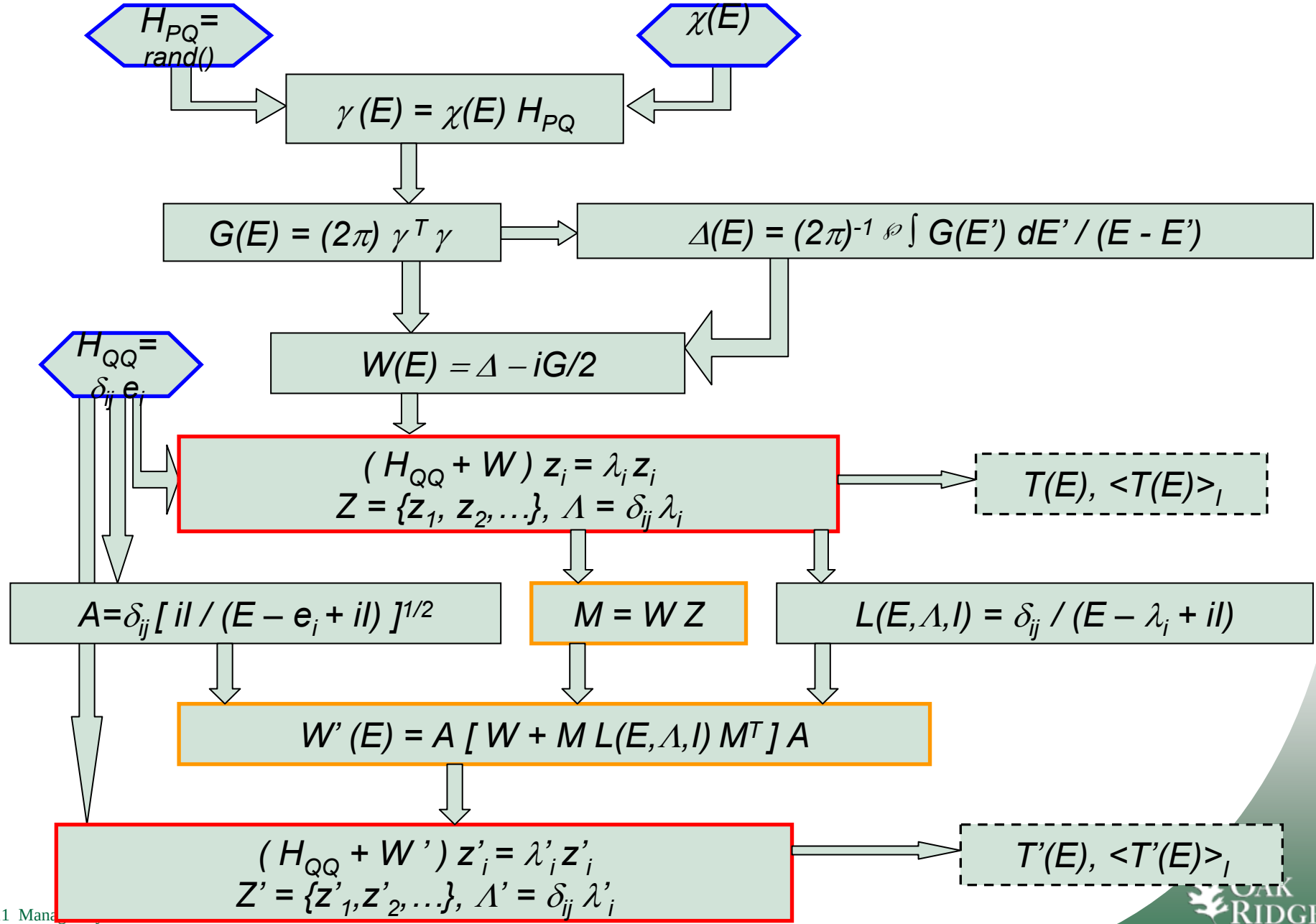
Cont'd. (1,600 Q-levels)

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

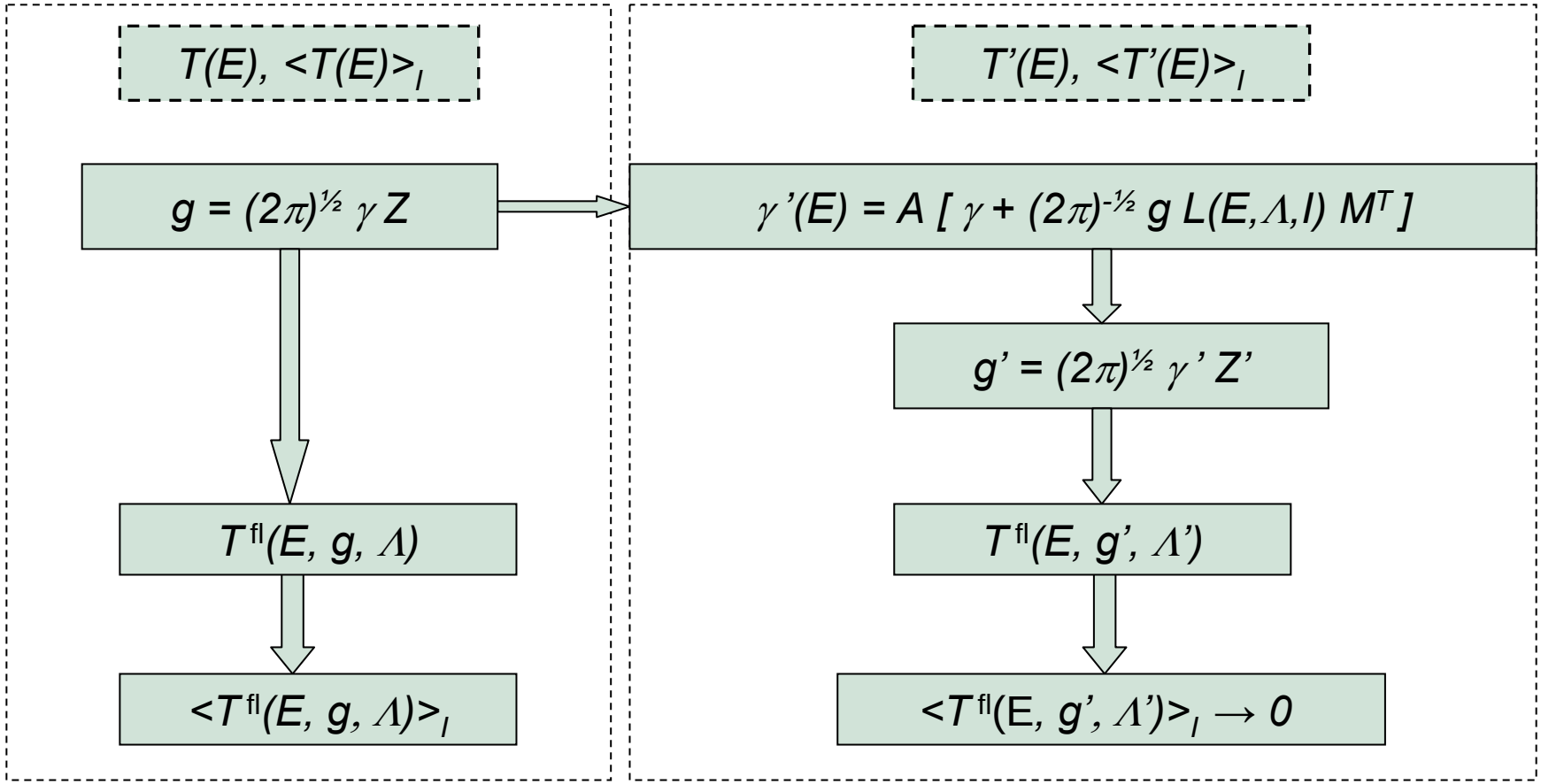




KKM Flowchart in matrix notation



KKM Flowchart cont'd



$$T^{fl}(E, g, \Lambda) \equiv (2\pi)^{-1}\, g\, L(E,\Lambda,0)\, g$$

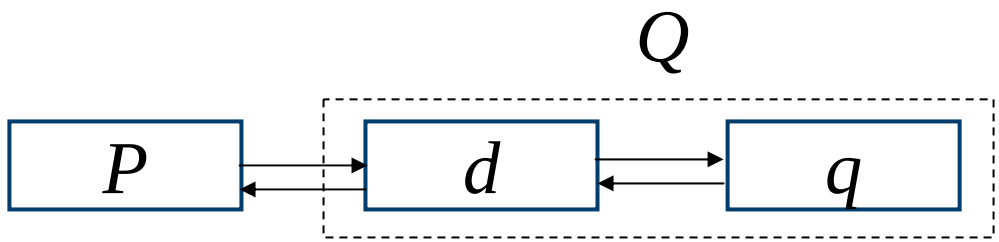
$$\langle T^{fl}(E, g, \Lambda)\rangle_l \equiv \int F_l(E - E')\, T^{fl}(E', g, \Lambda)\, dE',$$

$$F_l(x) = (l/\pi)/(x^2+l^2)$$

KKM extended to intermediate structure

Feshbach, Kerman, and Lemmer
Ann. of Phys. 41, 230 (1967)

- **T-matrix has three components:**
  - **Direct ("P")**
  - **Doorway ("d")**
  - **Resonant ("q")**



$$T = T^{\mathrm{dir}} + T^{d} + T^{\mathrm{res}}$$

$$\langle T \rangle_{I_{\mathrm{int}}} = T^{\mathrm{dir}} + T^{d} + \langle T^{\mathrm{res}} \rangle_{I_{\mathrm{int}}}$$

$$T = T^{\mathrm{int}} + T_{d}^{\mathrm{fl}}$$

$$\langle T \rangle_{I_{\mathrm{int}}} = T^{\mathrm{int}} \quad \Rightarrow \quad \langle T_{d}^{\mathrm{fl}} \rangle_{I_{\mathrm{int}}} \approx 0$$

- **Energy average over** $I_{\mathrm{int}} < \Gamma_{d}$
  - **"intermediate" structure**
  - **Finer than "gross", but coarser than "fine" structure**

This is a novel formal result, that will be tested by our parallel code.

This simplifies cross section: $\langle \sigma \rangle_{I_{\mathrm{int}}} \sim \langle |T|^{2} \rangle_{I_{\mathrm{int}}}$

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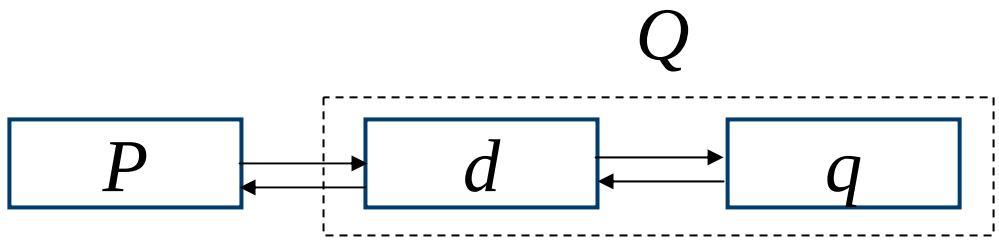

$$T = T^{\text{int}} + T_d^{\text{fluct}} \quad ,$$

$$T_{cc'}^{\text{int}} \equiv \left\langle \phi_c \left| V^{\text{int}} \right| \Psi_{c'}^{\text{int}} \right\rangle,$$

$$(E - H_{PP}^{\text{int}})\Psi_{c'}^{\text{int}} = 0$$

$$T_{cc'}^{\text{fluct}} \equiv \frac{1}{2\pi} \sum_q \frac{g_{cq} g_{c'q}}{E - \varepsilon_q},$$

$$g_{cq} = \sum_d \frac{g_{cd} g_{dq}}{E - \varepsilon_d}$$

KKM Summary II

- **From the Fluctuating T-matrix, KKM *derived* an energy averaged cross section in terms of optical potential transmission coefficients = *modified Hauser-Feshbach***
  - ***Energy averaging interval* = I, s.p. state width, 0.5 MeV**
  - **"gross" structure**

$$\langle \sigma^{\mathrm{fl}}_{cc'} \rangle_I \sim X_{cc} X_{c'c'} + X_{cc'} X_{c'c} \qquad X_{cc'} = \left\langle g_{cq} g^{*}_{c'q} \right\rangle_I$$

$$\langle \sigma^{\mathrm{fl}}_{cc'} \rangle_I \sim \frac{1}{\sum P_{c''}} \{ P_{cc} P_{c'c'} + P_{cc'} P_{cc'} + \ldots \}$$

$$P_{cc'} = (1 - \overline{S}\,\overline{S}^{*})_{cc'} = X_{cc'} Tr(X) + (X^2)_{cc'}$$

General computational issues

- **Finding Eigenvalues/vectors of large complex symmetric matrices**
  - **May be relevant to Gamow Shell Model**
- **Matrix product of large matrices**
- **User friendly parallelization of the above using K. Roche programming interface**

Intermediate structure transmission coeff.'s

- **From the Fluctuating T-matrix, an "intermediate" energy averaged cross section in terms of intermediate transmission coefficients**
  - ***Energy averaging interval*** **= I_{int} < doorway state width, 0.1 MeV**
  - **"intermediate" structure**

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

$$\langle \sigma_{cc'}^{\text{fl}} \rangle_{I_{\text{int}}} \sim \frac{1}{\sum P_{c''c''}^{\text{int}}} \left\{ P_{cc}^{\text{int}} P_{c'c'}^{\text{int}} + P_{cc'}^{\text{int}} P_{cc'}^{\text{int}} + \ldots \right\}$$

$$P_{cc'}^{\text{int}} = (1 - \overline{S}^{\text{int}} \overline{S}^{\text{int}*})_{cc'} = X_{cc}^{\text{int}} Tr(X^{\text{int}}) + (X^{\text{int}} X^{\text{int}})_{cc'}$$

- **The above can be generalized to even finer energy structures, as long as many compound levels ("q") are contained in the energy averaging interval.**

2009 Accomplishments

- **The KKM algorithm was rewritten following the M. Schwartz B.Sc. Thesis (1972, Prof. Kerman)**
  - **More efficient matrix operations**
  - **Alternative implementation of the Green's function**
- **Implemented the KKM algorithm in parallel in C:**
  - **parallelized complex-symmetric eigensolver**
  - **parallelized matrix multiplication**
  - **Much larger density of compound states accessible**
- **Extended the KKM theory beyond optical model:**
  - **doorway states, hallway states …**
  - **Not yet implemented numerically**

Remaining tasks for this year

- **Benchmark parallel KKM runs**
  - **Explore the limits of the matrix size**
- **Implement the KKM formalism for doorway states**
  - **Attempt to reproduce the intermediate structure c.s. of medium mass nuclei.**

Plan for the next year

- **Make the code robust**
- **Extend the parallel code to explore the approximations in the KKM cross section, and its offshoots (as many as possible):**
  - **Kerman-McVoy two-step reactions**
  - **Feshbach-Kerman-Koonin multistep reactions**
  - **Kerman-Sevgen statisical relations**
- **Feshbach-Kerman-Lemmer doorway states**
  - **in conjuction with the above**