

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

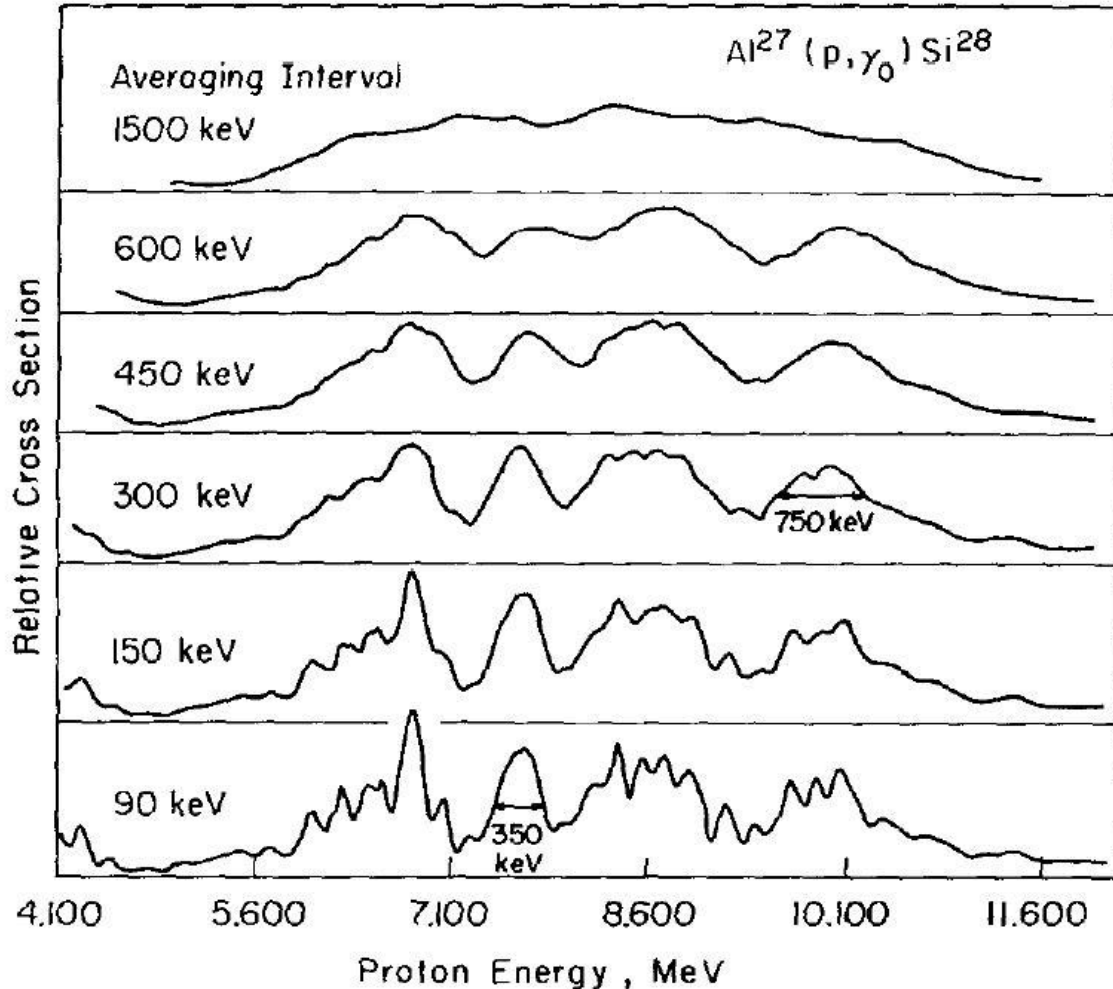
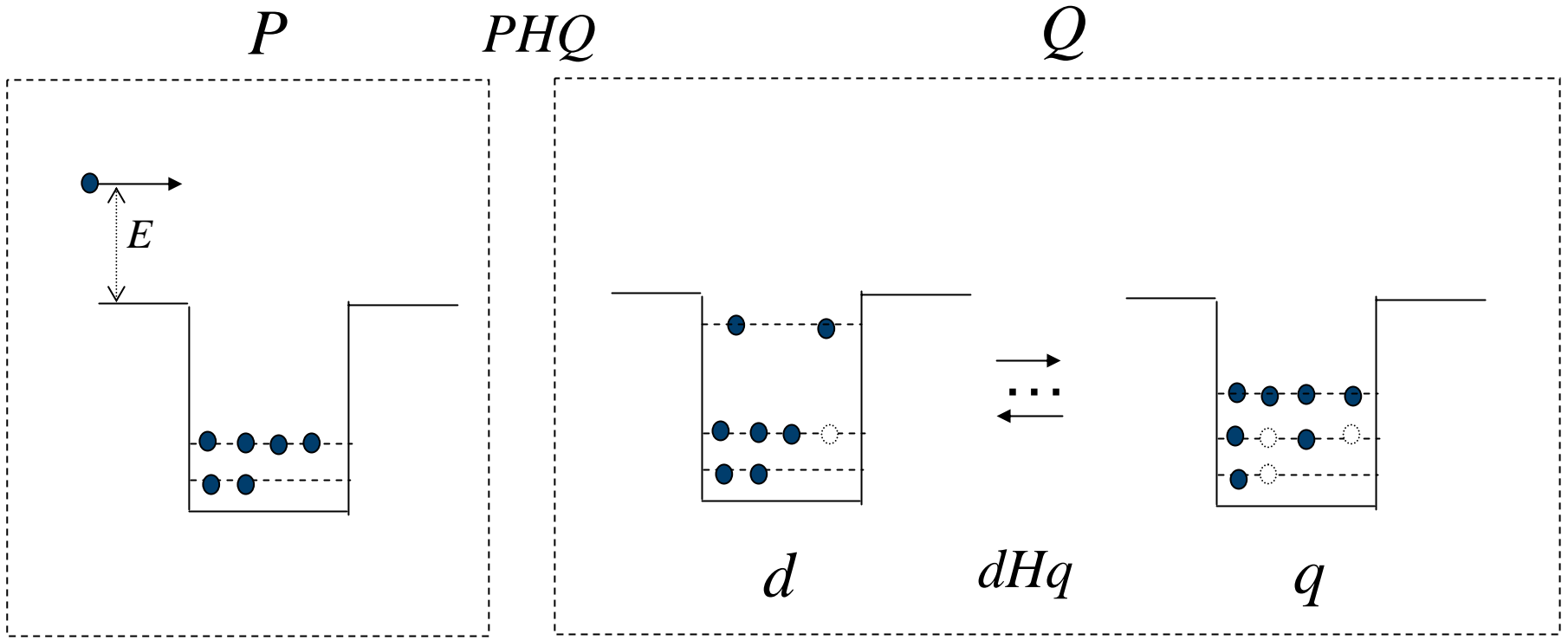


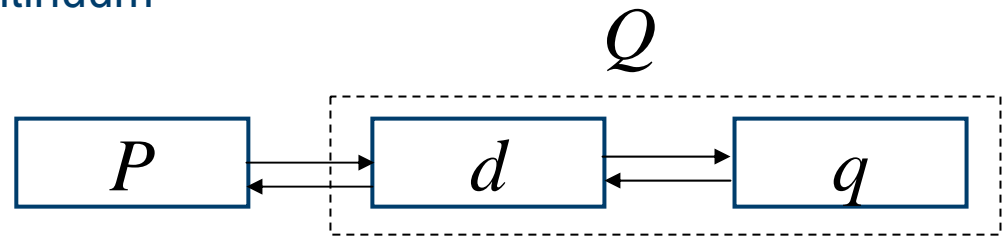
FIG. 6. Photocapture of protons by Al^{27} to the ground state of Si^{28} . The data is presented for various stages of resolution. From ref. 26.

Physical picture

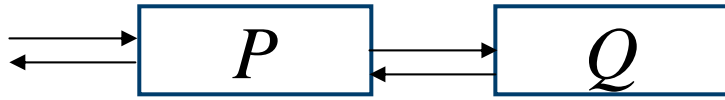


continuum

bound



KKM Introduction



Projection operators:

P – continuum space projection operator

Q – compound space projection operator

$$H\Psi = E\Psi$$

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

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

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

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

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

$$\Rightarrow T = T^{\text{dir}} + \langle \chi | H_{PQ} \frac{1}{E - H_{QQ} - H_{QP} \frac{1}{E - H_{PP}} H_{PQ}} | \chi \rangle$$

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

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

KKM Introduction

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

$$\begin{aligned} [H_{QQ} + H_{QP} G_P H_{PQ}] | \hat{q} \rangle &= \hat{\mathcal{E}}_q | \hat{q} \rangle \\ \langle \tilde{q} | [H_{QQ} + H_{QP} G_P H_{PQ}] &= \langle \tilde{q} | \hat{\mathcal{E}}_q \end{aligned}$$

$$\begin{aligned} \hat{\mathcal{E}}_q &= \hat{E}_q - i \frac{\hat{\Gamma}_q}{2} & H_{QQ} | Q_j \rangle &= E_{Q_j} | Q_j \rangle \\ \sum_{\hat{q}} | \hat{q} \rangle \langle \tilde{q} | &= 1 & \sum_j | Q_j \rangle \langle Q_j | &= 1 \\ \langle \tilde{q} | \hat{q}' \rangle &= \delta_{\hat{q}\hat{q}'} & \langle Q_j | Q_j \rangle &= \delta_{ij} \end{aligned}$$

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

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

Matrix size limited by the eigensolver:
 1 CPU < 10⁴,
 in parallel < 10⁶

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)

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

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

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

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

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

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

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”)

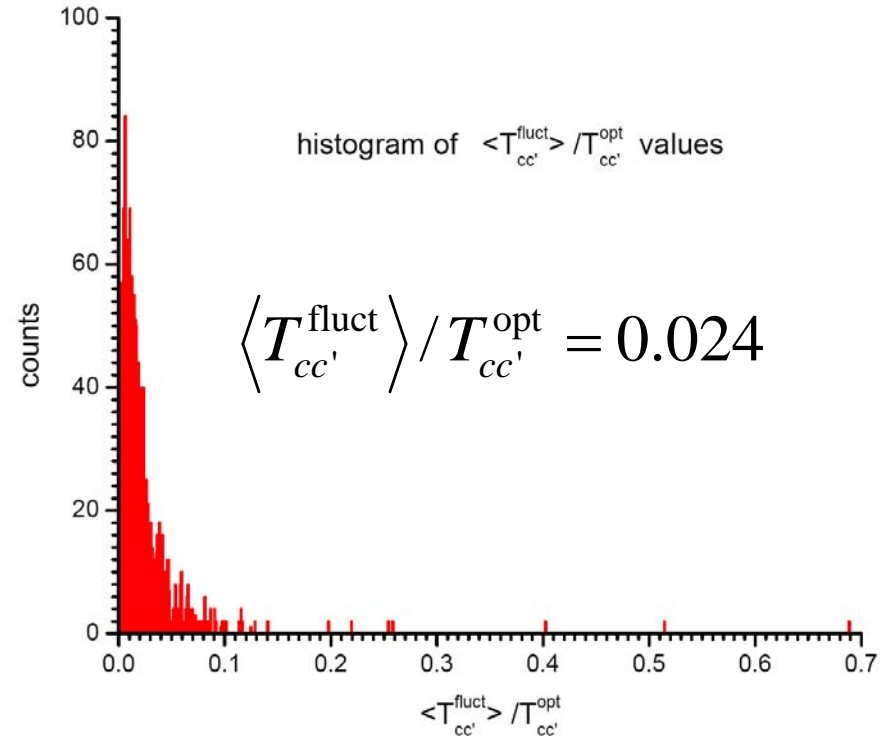
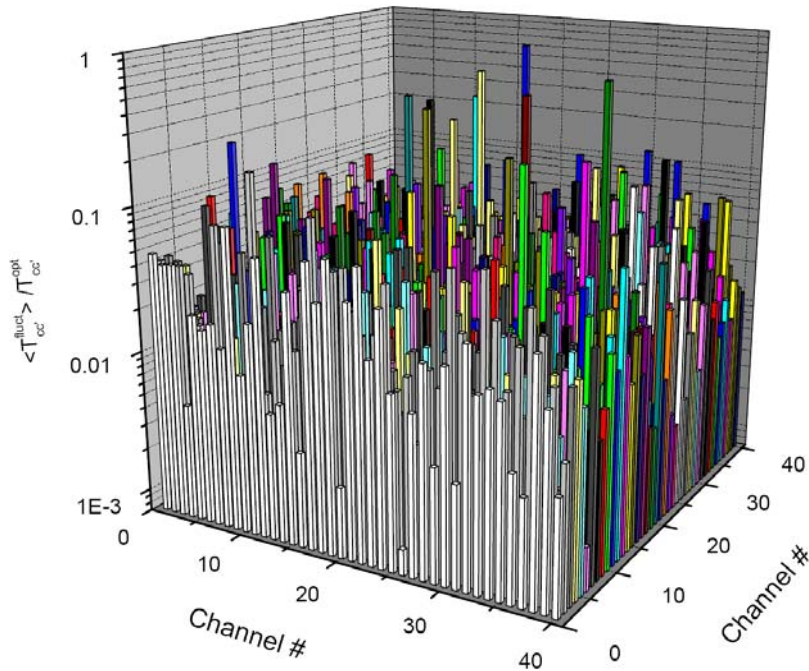
- **KKM Two-pot. T-matrix:**
 - Optical (“opt”)
 - Fluctuating (“fl”)

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

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

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

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



Computation parameters:

- 400 equidistant Q-levels
- 40 channels
- 20 equidistant radial points where H_{PQ} set to a Gaussian-distributed random

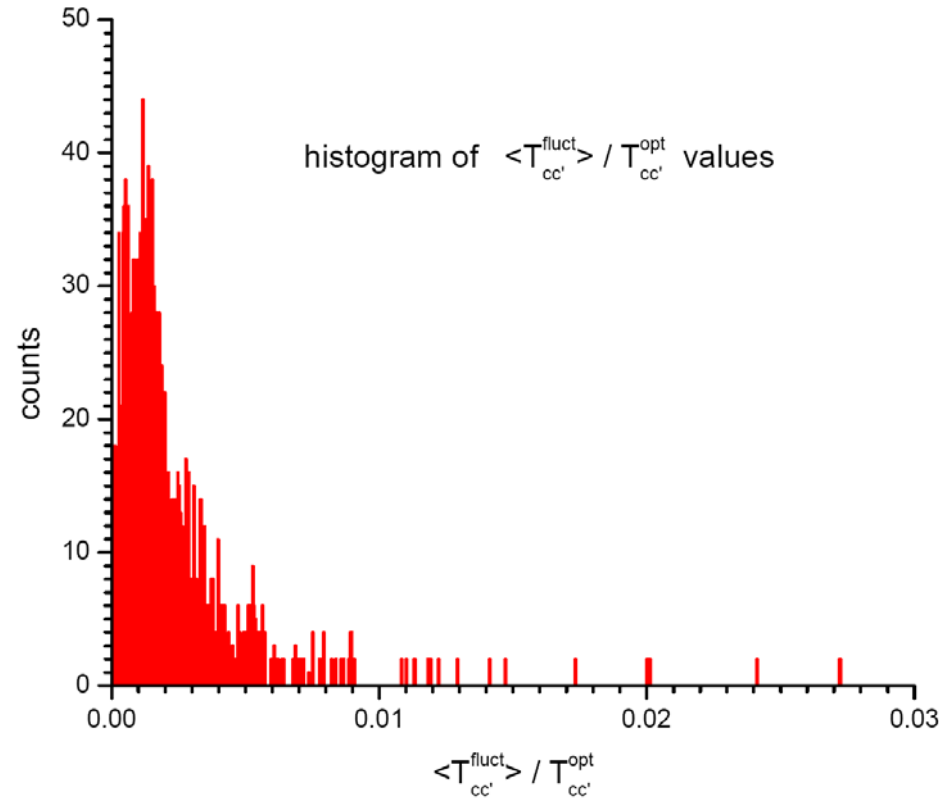
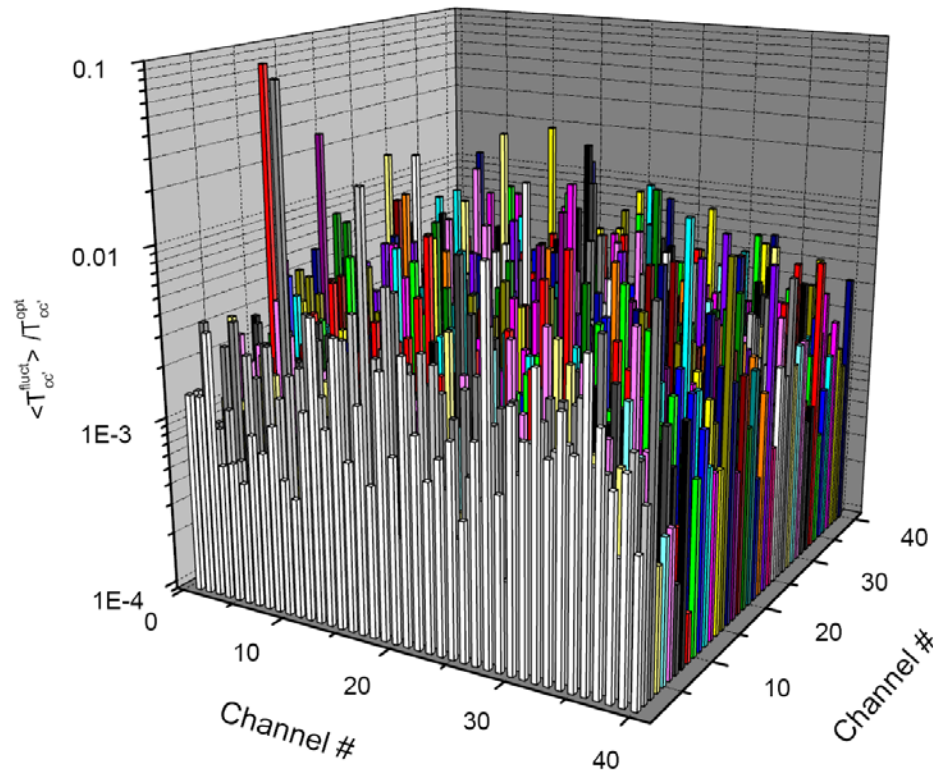
interaction

- $E = 20$ MeV
- 100 E' points for Lorentzian averaging between 18 and 22 MeV
- $I = 0.5$ MeV
- s-wave only
- $\Gamma/D \gg 1$

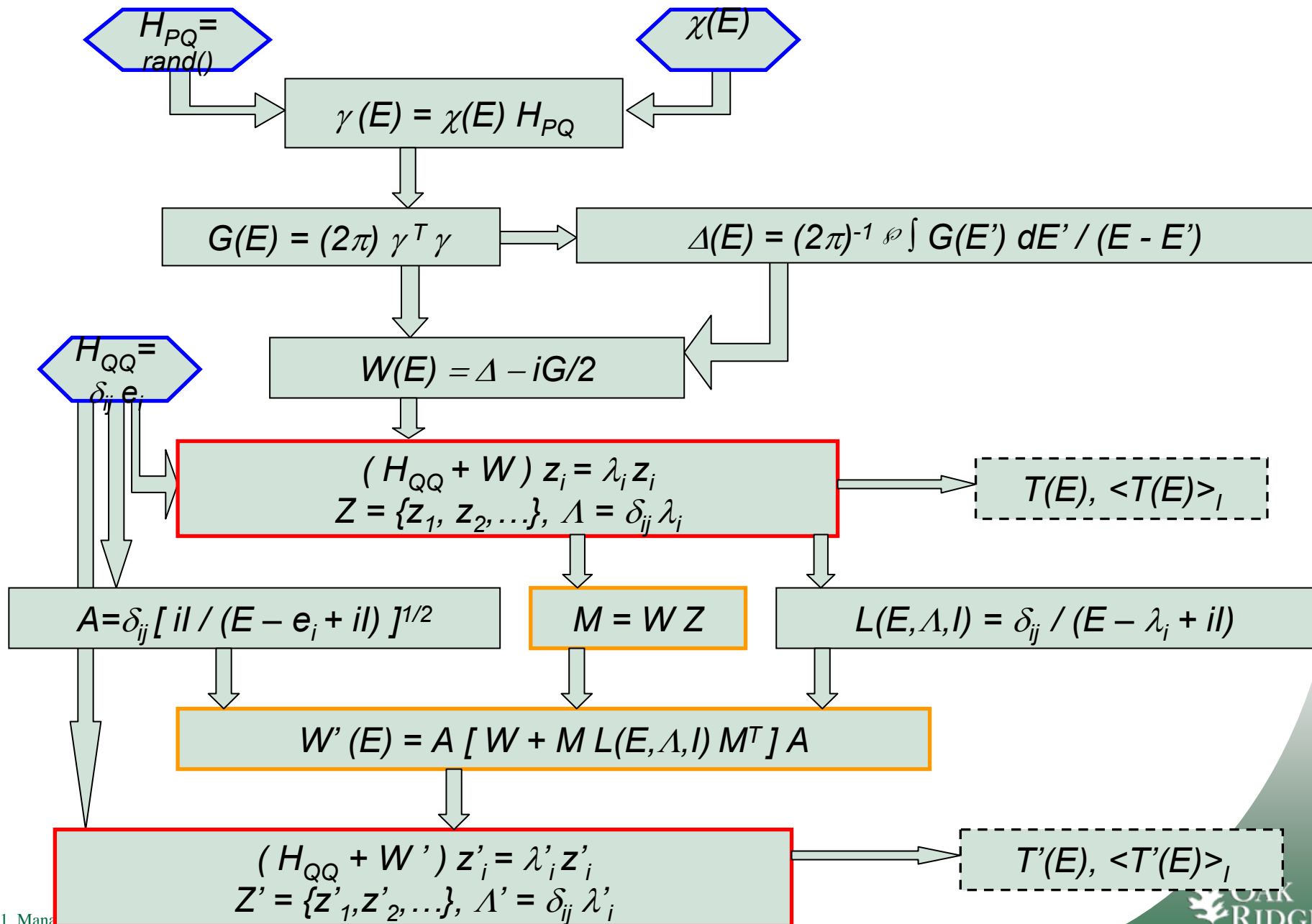
In the spirit of:
Dagdeviren and Kerman,
Ann. of Phys. **163** (1985) 199

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

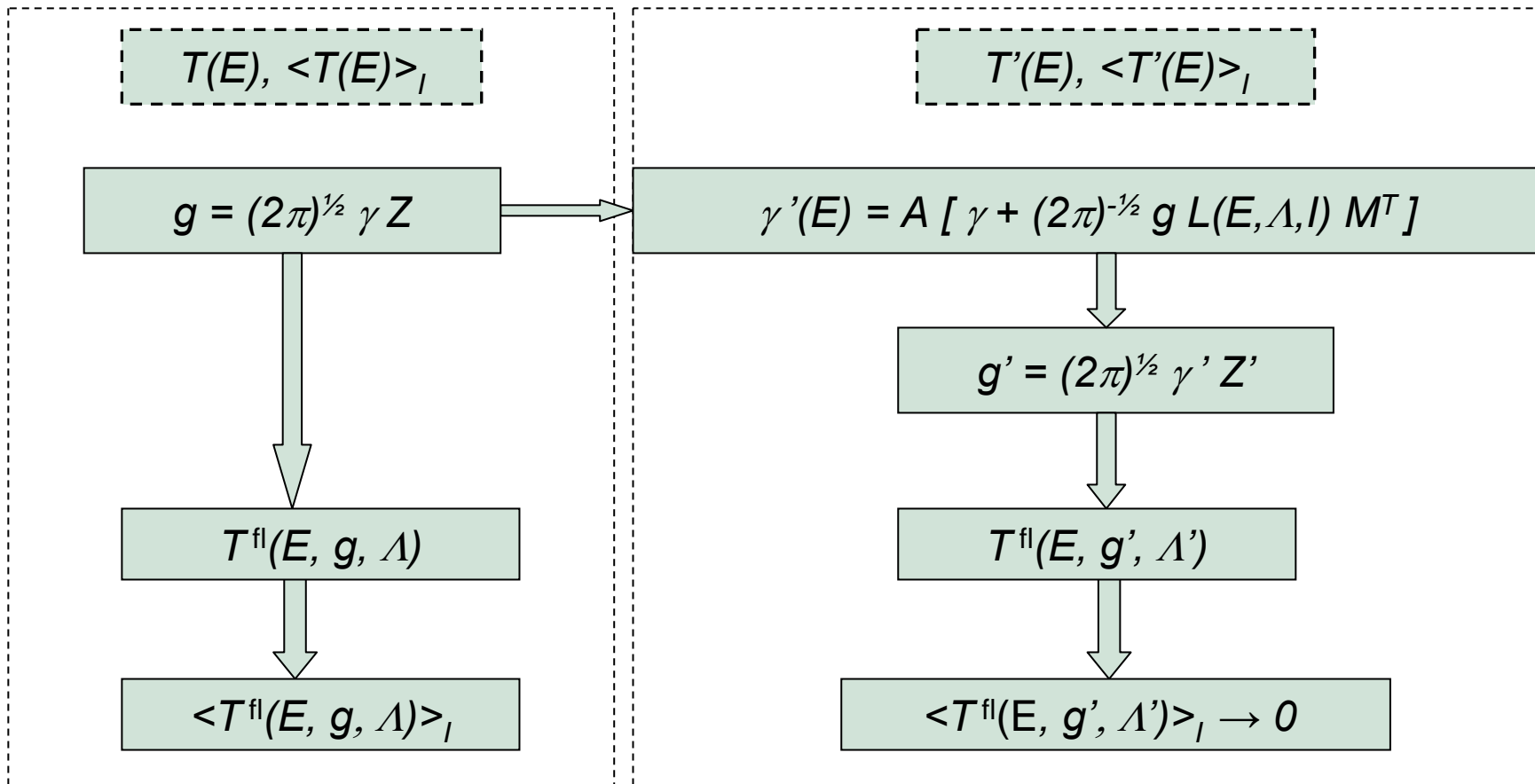
$$\left\langle \left\langle T_{cc'}^{\text{fluct}} \right\rangle / T_{cc'}^{\text{opt}} \right\rangle = 0.0024$$



KKM Flowchart in matrix notation



KKM Flowchart cont'd



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

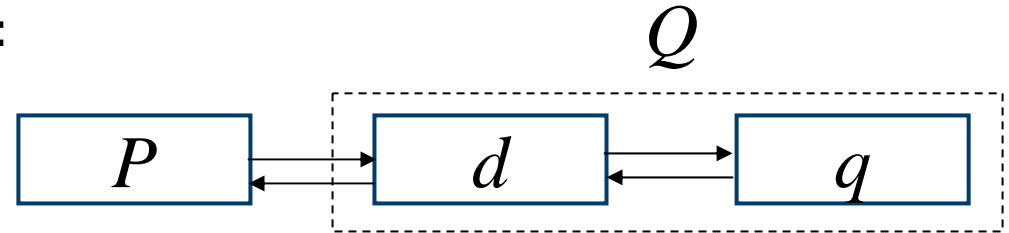
$$\langle T^{fl}(E, g, \Lambda) \rangle_I \equiv \int F_I(E - E') T^{fl}(E', g, \Lambda) dE',$$

$$F_I(x) = (I/\pi)/(x^2 + I^2)$$

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”)



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

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

$$T = T^{\text{int}} + T_d^{\text{fl}}$$

$$\langle T \rangle_{I_{\text{int}}} = T^{\text{int}} \Rightarrow \langle T_d^{\text{fl}} \rangle_{I_{\text{int}}} \approx 0$$

- **Energy average over $I_{\text{int}} < \Gamma_d$**
 - “intermediate” structure
 - Finer than “gross”, but coarser than “fine” structure

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

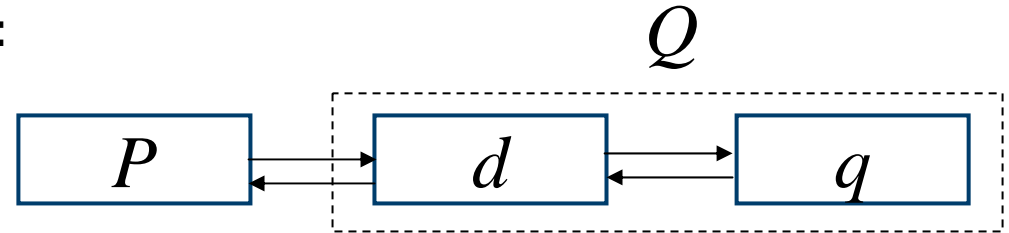
This simplifies cross section: $\langle \sigma \rangle_{I_{\text{int}}} \sim \langle |T|^2 \rangle_{I_{\text{int}}}$

KKM extended to intermediate structure

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- **T-matrix has three components:**

- Direct (“P”)
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$$T = T^{\text{int}} + T_d^{\text{fluct}},$$

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

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

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

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

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

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

$$\langle \sigma_{cc'}^{\text{fl}} \rangle_I \sim \frac{1}{\sum P_{c''}} \{ P_{cc} P_{c'c'} + P_{cc'} P_{cc'} + \dots \}$$

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

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 = $I_{\text{int}} <$ doorway state width, 0.1 MeV
 - “intermediate” structure

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

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

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

- 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 statistical relations**
- **Feshbach-Kerman-Lemmer doorway states**
 - **in conjunction with the above**