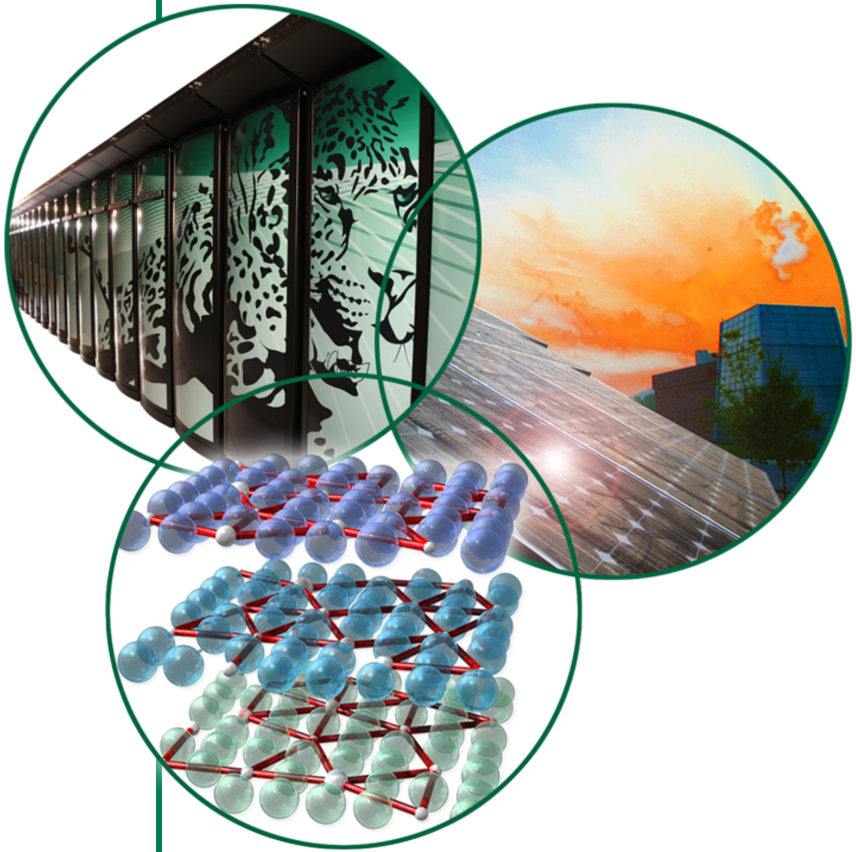
Extending the Kawai-Kerman-McVoy Statistical Theory of Nuclear Reactions to Doorway States



Nuclear Data Week, BNL

November 14-18, 2011

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U.S. DEPARTMENT OF ENERGY

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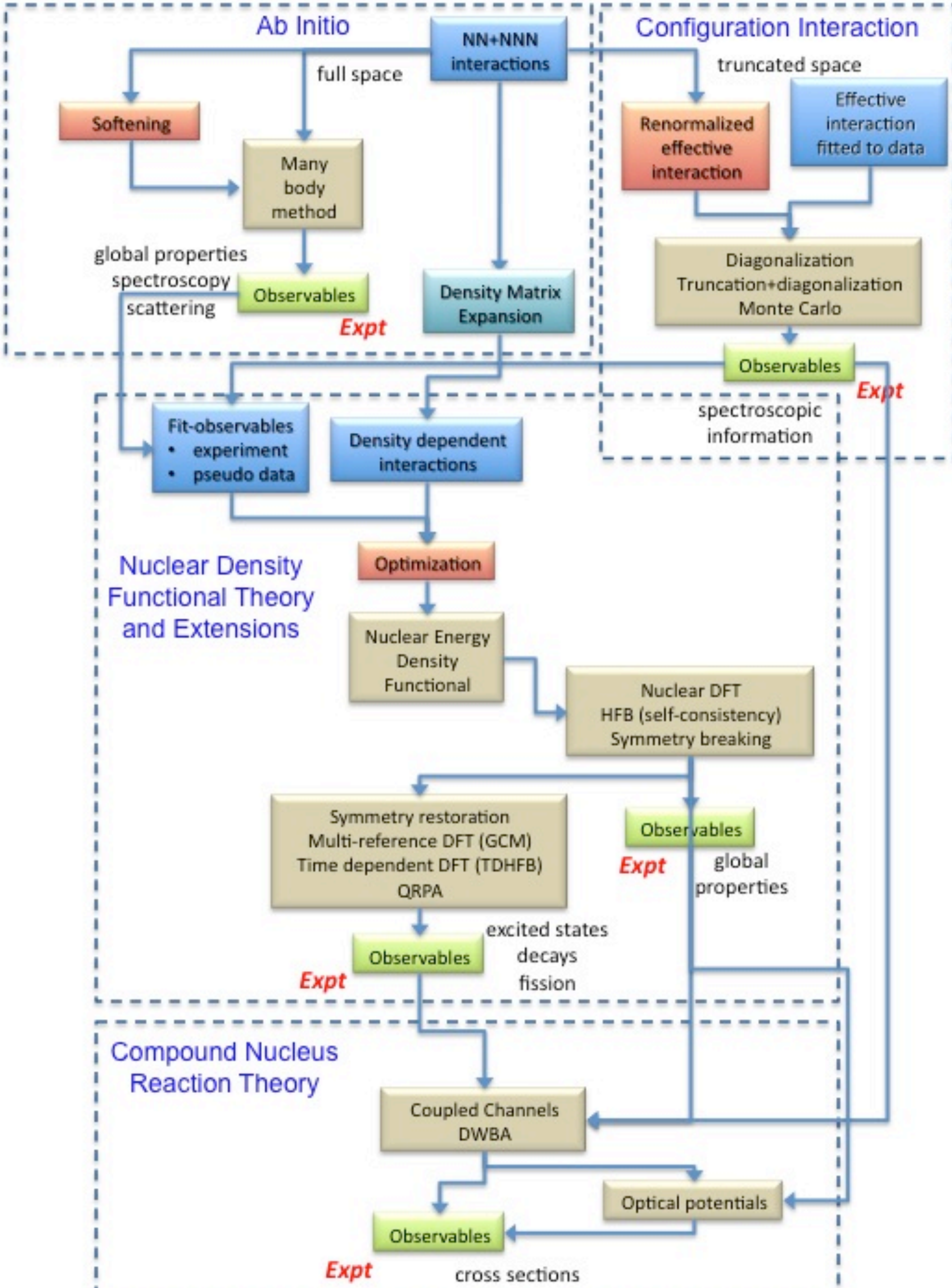

- **UNEDF SciDAC:**
- **www.unedf.org**

HPC numerical simulation of formal theories of statistical nuclear reactions

Energy structures in cross sections

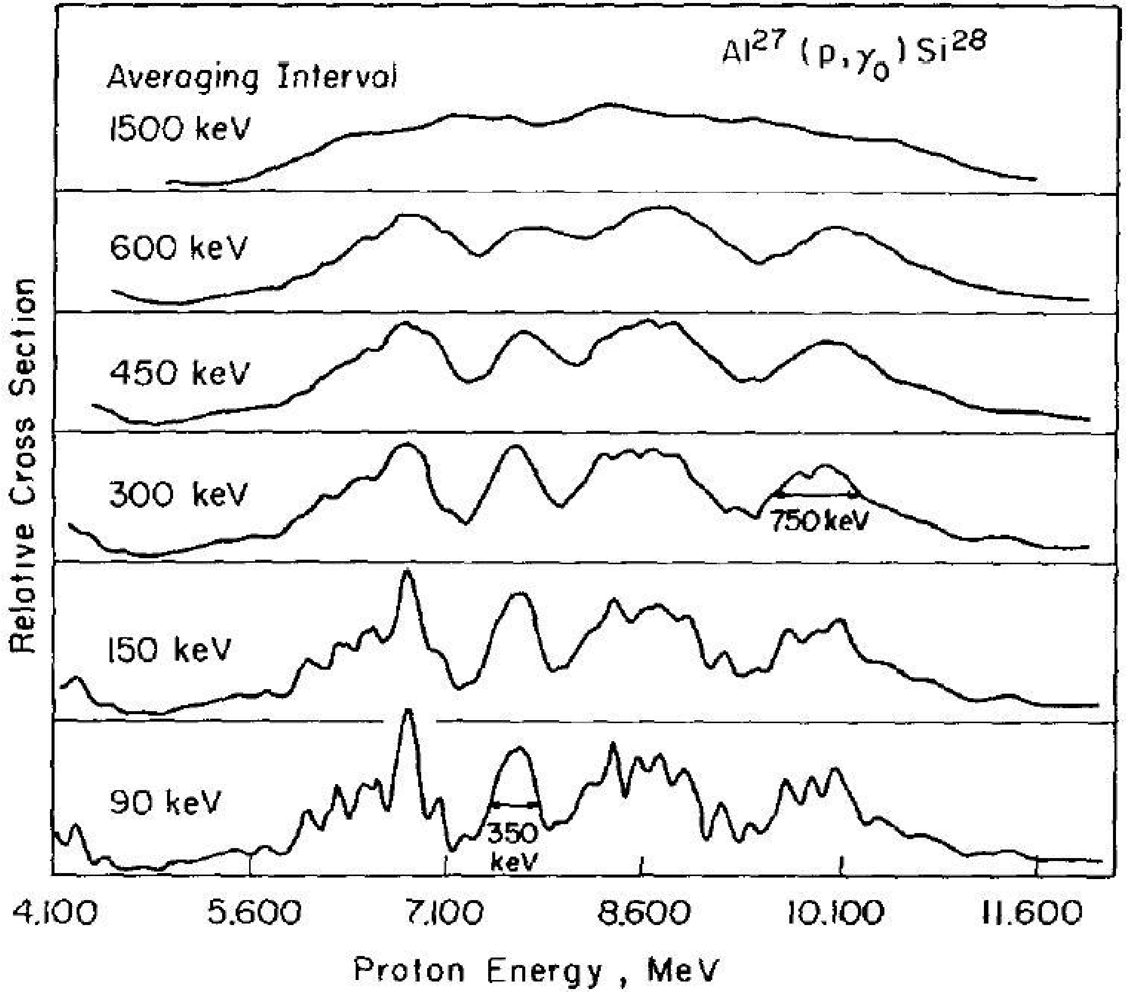

FIG. 6. Photocapture of protons by Al^{27} to the ground state of Si^{28}. The data is presented for various stages of resolution. From ref. 26.

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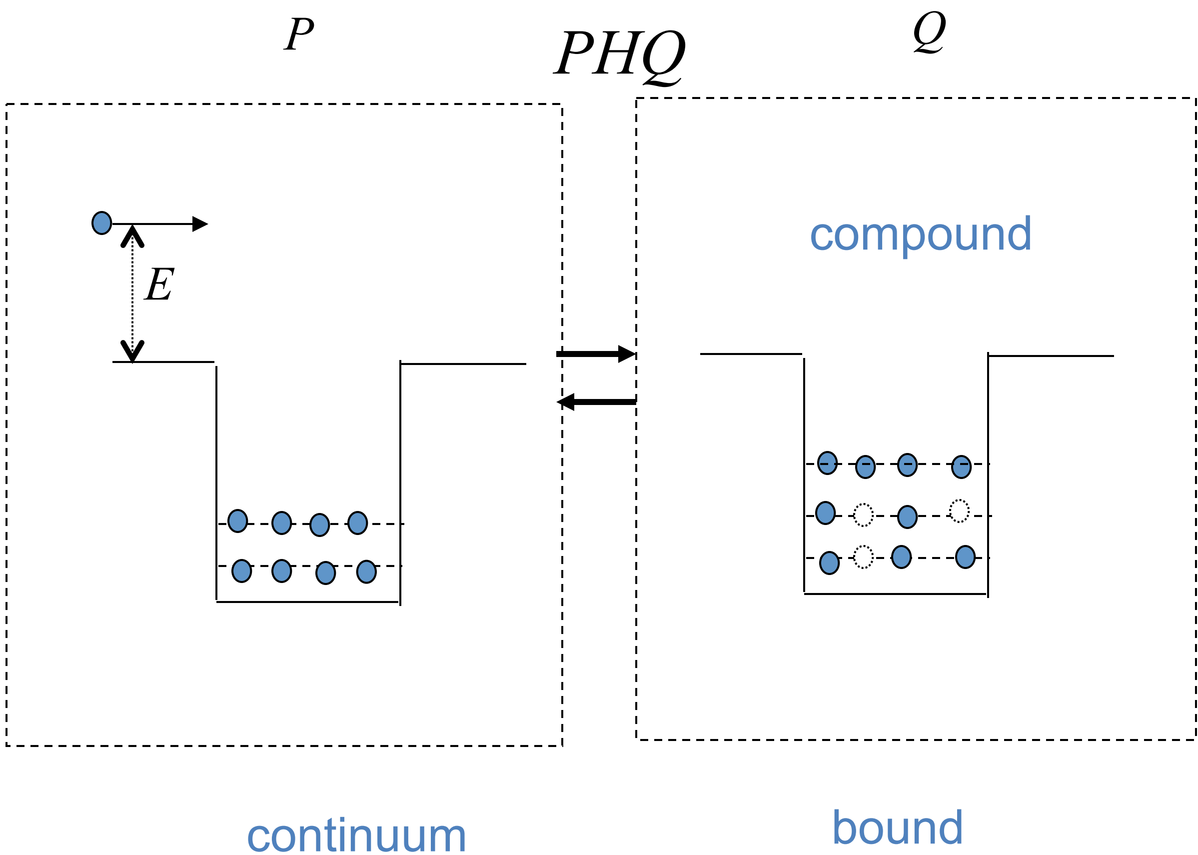
Presentation_name

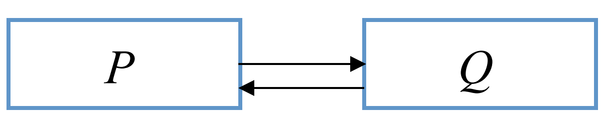
Why KKM?

- A framework based on Feshbach's projection operators
- Central result:
  - $T = T_{background} + T_{resonant} = T_{average} + T_{fluctuating}$
- A foundation for derived statistical theories:
  - Kerman-McVoy
    - Designed for two step processes like A(d,p)B*, B*→A+n
    - Could be used for statistical (d,p) reactions at FRIB
    - Accounts for doorway states (IAR)
  - Feshbach-Kerman-Koonin (FKK)
    - Multistep reactions (doorway, hallway, etc.), used for nuclear data analysis
- Expressions similar to KKM were derived by other methods
  - Random Matrix Theory
  - Maximum Entropy Method

Kawai-Kerman-McVoy:

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





Feshbach's projection operators

$$H\Psi = E\Psi$$

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

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

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

Two-potential formula yields

$$\Rightarrow \quad T = \langle \phi | V_{PP} | \chi \rangle + \langle \chi | H_{PQ} \frac{1}{E - H_{QQ} - H_{QP} \frac{1}{E - H_{PP}} H_{PQ}} H_{QP} | \chi \rangle$$

$$\equiv T_{\text{background}} + T_{\text{resonant}}$$

KKM Fluctuation T-matrix

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

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

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

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

Two-potential formula yields

$$\Rightarrow \quad T = \langle \phi | H_{\text{opt}} | \bar{\Psi} \rangle + \langle \bar{\Psi} | V_{PQ} \frac{1}{E-H_{QQ}-V_{QP}\frac{1}{E-H_{\text{opt}}}V_{PQ}} V_{QP} | \bar{\Psi} \rangle$$

$$\equiv T_{\text{optical}} + T_{\text{fluctuation}}$$

$$\Rightarrow \quad \langle T_{\text{fluctuation}} \rangle \approx 0$$ **is the central result of the KKM**

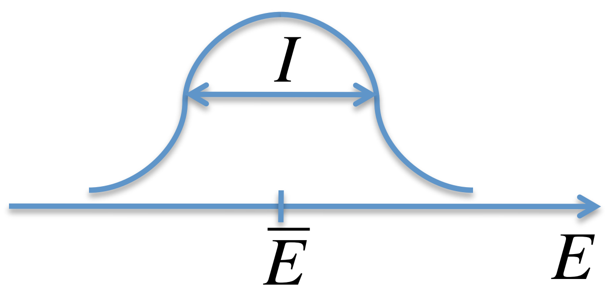
$$\Rightarrow \quad \langle \sigma \rangle \approx \sigma_{\text{optical}} + \langle \sigma_{\text{fluctuation}} \rangle$$

Expand the T-matrix by eigenfunctions

$$T_{cc'}^{\text{fluct}}(E) \equiv \frac{1}{2\pi}\sum_q \frac{g_{cq}(E)g_{c'q}(E)}{E-\mathcal{E}_q(E)}$$

$$g_{cq}(E) = \sum_Q \langle \psi_c(E) | V_{cQ}(E) | Q \rangle \langle Q | q(E) \rangle$$

This E-dependence now treated explicitly.

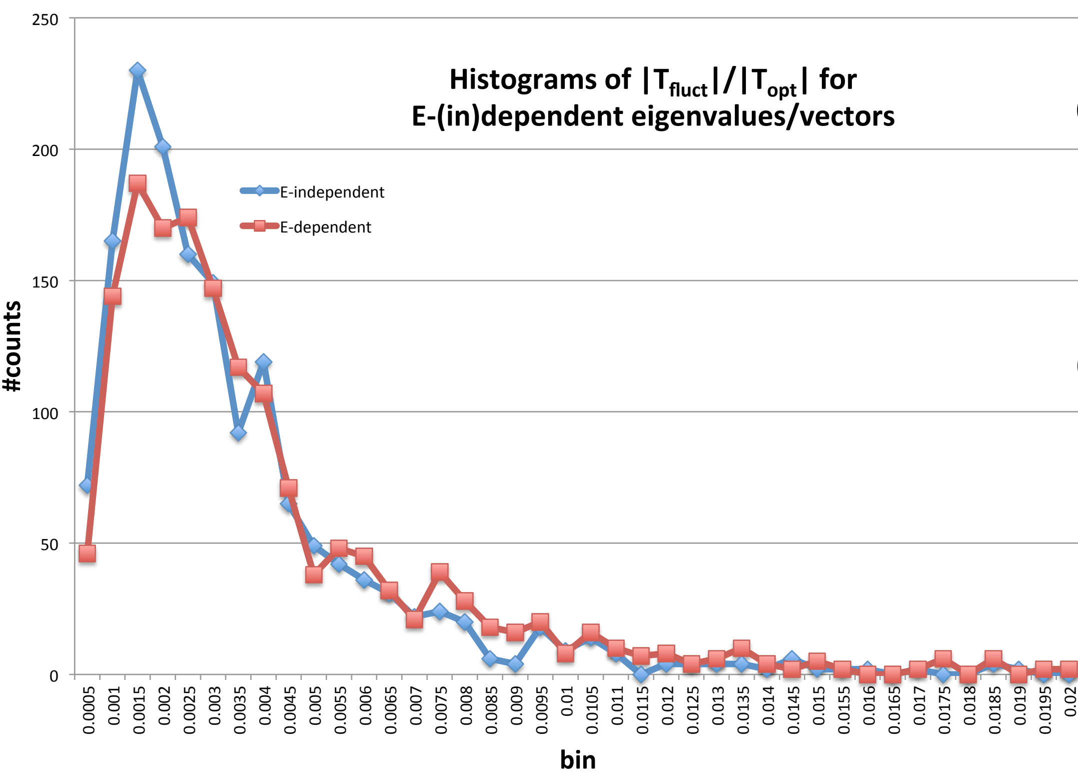


Lorentzian weight function width I.

$$\left\langle T_{cc'}^{\text{fluct}}(E) \right\rangle_I \equiv \frac{I}{2\pi}\int \frac{dE'}{(E-E')^2 + \frac{I^2}{4}} T_{cc'}^{\text{fluct}}(E') \quad \approx \quad 0 \ ?$$

Results:

Eigenvalues/vectors	Average Ratio	SQRT(Variance)
E-independent	0.0037	0.0053
E-dependent	0.0042	0.0049



Computation parameters:

- Eigenvalues/vectors computed at 100 energies spanning 18-22 MeV
- 1600 equidistant Q-levels
- 40 channels
- 20 equidistant radial points where H_{PQ} drawn from a Gaussian-distributed random interaction
- E = 20 MeV
- 100 E' points for Lorentzian averaging between 18 and 22 MeV
- Lorentzian averaging width I = 0.5 MeV
- s-wave only
- Strongly overlapping resonances

Test approximations in KKM derivation

- **The E-dependence makes E-averaging more accurate**

$$T_{cc'} = \overline{T}_{cc'} + \frac{1}{2\pi}\sum_q \frac{g_{qc}(E)g_{qc'}(E)}{E-\mathcal{E}_q(E)} = \overline{T}_{cc'} + T_{cc'}^{\text{fluct}}$$

$$\Rightarrow \left\langle \sigma_{cc'}^{\text{fluct}} \right\rangle \sim \left\langle \left| T_{cc'}^{\text{fluct}} \right|^2 \right\rangle_I$$

Random Phase Hypothesis

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

Preliminary results are analyzed.

$$\cong 2\pi \left\langle \frac{g_{qc}g_{qc'}g_{qc}^* g_{qc'}^*}{D_q \Gamma_q} \right\rangle_q$$

$$\cong \frac{2\pi}{D_q \Gamma_q} \left\langle g_{qc}g_{qc'}g_{qc}^* g_{qc'}^* \right\rangle_q$$

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

KKM Cross Section (Transmission Coeff.)

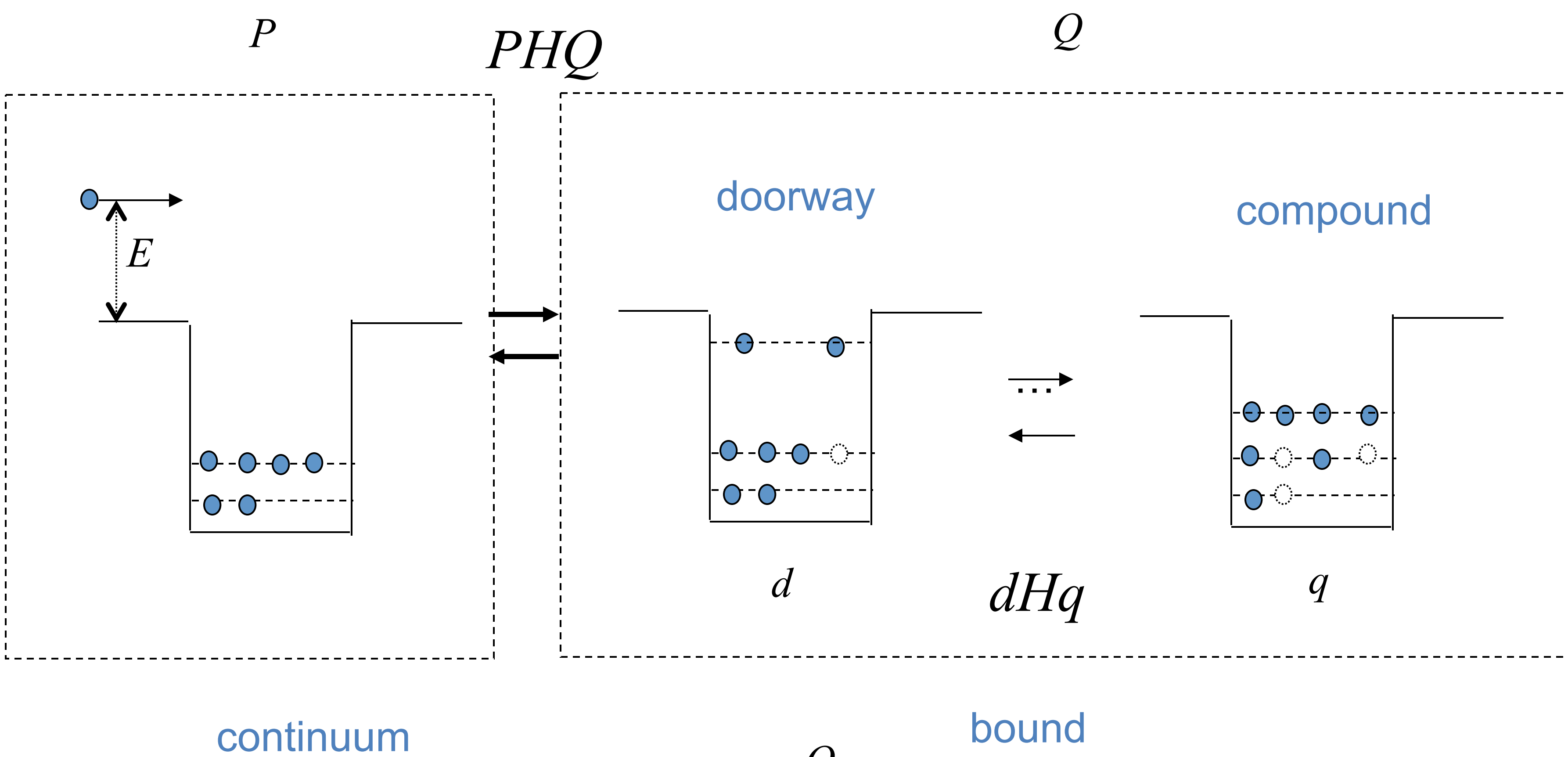
- **From the Fluctuating T-matrix, KKM *derived* an energy averaged cross section in terms of optical potential transmission coefficients = *modified Hauser-Feshbach***
  - ***Energy averaging interval* = I, s.p. state width, 0.5 MeV**
  - **"gross" structure**

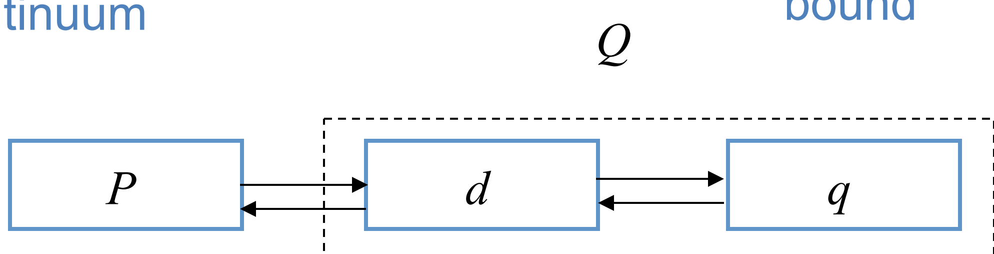
$$\langle \sigma^{\mathrm{fl}}_{cc'} \rangle_I \sim X_{cc} X_{c'c'} + X_{cc'} X_{c'c} \qquad X_{cc'} = \left\langle g_{cq} g^*_{c'q} \right\rangle_I$$

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

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

Doorway states in the KKM theory

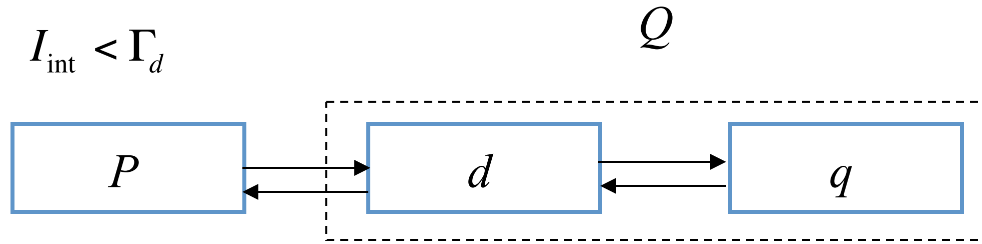




KKM extended to intermediate structure

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

$I_{\text{int}} < \Gamma_d$



$$T = T^P + T^d + T^q(E) \quad \Leftrightarrow \quad T = T^P + T^Q(E)$$

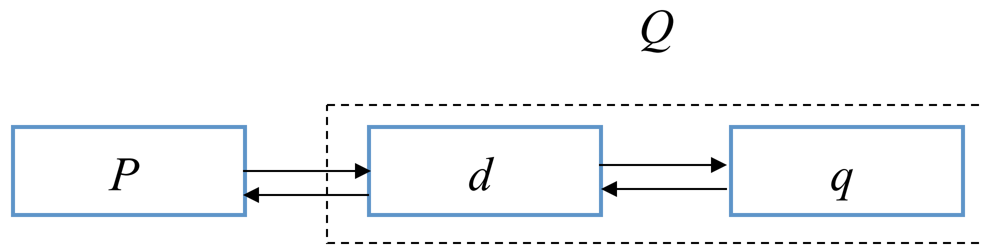
$$T = T^{\text{int}} + T_q^{\text{fluct}}(E) \quad \overset{?}{\Leftrightarrow} \quad T = T^{\text{opt}} + T_Q^{\text{fluct}}(E)$$

$$T_q^{\text{fluct}}(E) = H_{Pd}\frac{1}{E - H_{dd} - W_{dd}} H_{dq} \frac{1}{E - H_{qq} - H_{qd}\dfrac{1}{E - H_{dd} - W_{dd}} H_{dq}} H_{qd} \frac{1}{E - H_{dd} - W_{dd}} H_{dP}$$

$$T_q^{\text{fluct}}(E) = \frac{1}{2\pi}\sum_q \frac{\gamma_{cq}(E)\gamma_{c'q}(E)}{E - \mathsf{E}_q(E)}, \qquad \gamma_{cq}(E) = \sum_d \frac{g_{cd}(E) g_{dq}(E)}{E - \mathsf{E}_d(E)}$$

KKM extended to intermediate structure

$$T = \langle T \rangle_{I_{\text{int}}} + T_q^{\text{fluct}}(E)$$



$$\langle T \rangle_{I_{\text{int}}} \approx T^{\text{int}}$$

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

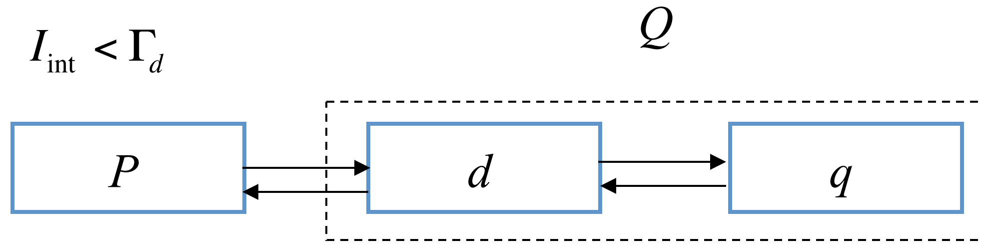
$$H^{\text{int}} = H_{PP} + H_{Pd} \frac{1}{E - H_{dd} - H_{dq} \dfrac{1}{E - H_{qq} + iI_{\text{int}}} H_{qd}} H_{dP}$$

$T = T^{\text{int}} + T_q^{\text{fluct}}(E)$ is analogous to $T = T^{\text{opt}} + T_Q^{\text{fluct}}(E)$

$$\langle T_q^{\text{fluct}}(E) \rangle_{I_{\text{int}}} \overset{?}{\approx} 0$$

KKM extended to intermediate structure

$$I_{\rm int} < \Gamma_d$$



$$T = T^P + T^d + T^q(E)$$

$$\langle T \rangle_{I_{\rm int}} = T^P + T^d + \langle T^q(E) \rangle_{I_{\rm int}}$$

$$T_q^{\rm fluct}(E) = T - \langle T \rangle_{I_{\rm int}}$$

$$= T^q(E) - \langle T^q(E) \rangle_{I_{\rm int}}$$

$$T^q(E) = \frac{1}{2\pi} \sum_q \frac{\gamma_{cq}(E)\gamma_{c'q}(E)}{E - E_q(E)}, \qquad \gamma_{cq}(E) = \sum_d \frac{g_{cd}(E) g_{dq}(E)}{E - E_d(E)}$$

$$\langle T^q(E) \rangle_{I_{\rm int}} = \frac{1}{2\pi} \sum_q \frac{\gamma_{cq}(E)\gamma_{c'q}(E)}{E - E_q(E) + iI_{\rm int}}$$

$$\frac{1}{E - E_q(E)} - \frac{1}{E - E_q(E) + iI_{\rm int}} = \frac{iI_{\rm int}}{(E - E_q(E))(E - E_q(E) + iI_{\rm int})}$$

$$T_q^{\rm fluct}(E) = \frac{1}{2\pi} \sum_q \frac{\bar{\gamma}_{cq}(E)\bar{\gamma}_{c'q}(E)}{E - E_q(E)}$$

$$\bar{\gamma}_{cq}(E) = \gamma_{cq}(E) \sqrt{\frac{iI_{\rm int}}{E - E_q(E) + iI_{\rm int}}}$$

$$T = \langle T \rangle_{I_{\rm int}} + T_q^{\rm fluct}(E)$$

- **Energy average over**
  - **"intermediate" structure**
  - **Finer than "gross", but coarser than "fine" structure**

Preliminary results for doorways

```
   nq =: 440, 840                NB. # of compound levels
   nd =: 60                      NB. # of doorway states
   strengthpd =: 0.05 0.005      NB. average coupling strength H_PD
   strengthdq =: 0.01 0.001      NB. average coupling strength H_DQ
   nc =: 20                      NB. # of channels
   ne =: 10                      NB. # of energy grid points
   radius =: 5.                  NB. radius of interaction
   nr =: 5                       NB. # of radial points in h(p,q,r)
   Elow =: 1.0                   NB. low end of the energy range
   Ehigh =: 2.0                  NB. high end of the energy range
   ii =: 0.05                    NB. energy averaging interval
   Echan_high =: 1.0             NB. nc equidistant channel
thresholds from 0 to Echan_high
```

nq	Avg(T_kkm)/Avg(T)	
	Non-overlapping res.'s	Overlapping res.'s
440	0.15	0.15
840	0.16	0.12

HPC progress report (by K. Roche)

- implemented novel parallel complex symmetric diagonalization routine in the spirit of ScaLAPACK
  - requires more extensive testing at scale
    - tested against zgeev()
    - self-consistent tests (|AZ-DZ|) (n= 65536)
    - against Toeplitz form (n=32768)

- implementation of triangular solves are one bottleneck that can be improved

- remove the kfil() data structures -stay incore

- plug in the parallel , parallel diagonalization routines over energies -code exists but we have not tested it
  - $E \sim E1, E2, \ldots, En$
  - instead of doing these in sequence, do them at once
    - form at most *n* subcommunicators of size $P*Q$; ($np \sim n * P * Q$) (P,Q are dimensions of virtual rectangular process grid)
    - perfect strong scaling over diagonalization phase in simple tests

Conclusions

- The effect of neglecting the E-dependence of eigenvalues and eigenvectors in the KKM is relatively small
- KKM derivation generalized to intermediate structure
  - Provides formal justification for faster E-dep. of optical potentials
  - May be generalized to finer structure:
    - Provided: there are many compound resonances in the E-averaging interval
  - The subtraction method could be used to simply derive the KKM

Outlook

- Complete *parallel* KKM with E-dep. eigenvalues/vectors
- Further testing of approximations in derivation of KKM cross sections is underway

Expand T-matrix in eigenvalues/vectors:

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

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

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

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

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

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

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

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

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

KKM subtraction

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

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

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

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

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

Energy averaging of the T-matrix yields this expression for optical potential and opt.w.f. (for Lorentzian averaging)

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

$$H_{\text{opt}} \equiv H_{PP} + H_{PQ}\frac{1}{E - H_{QQ} + iI} H_{QP}$$

Use H_{opt} to rewrite Eq. (3)

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

$$= \boxed{H_{PQ}\sqrt{\frac{iI}{E - H_{QQ} + iI}}}\,\frac{1}{E - H_{QQ}}\,\boxed{\sqrt{\frac{iI}{E - H_{QQ} + iI}}\,H_{QP}}\,P\Psi$$

$$\equiv V_{PQ}\frac{1}{E - H_{QQ}} V_{QP}P\Psi$$

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

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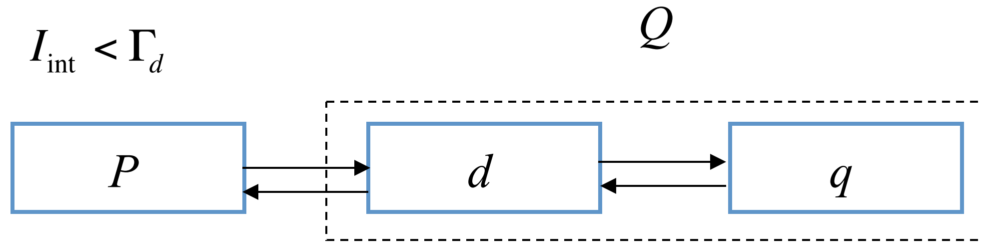
$I_{\text{int}} < \Gamma_d$



$$T = T^P + T^d + T^q(E) \quad \Leftrightarrow \quad T = T^P + T^Q(E)$$

$$T = T^{\text{int}} + T_q^{\text{fluct}}(E) \quad \overset{?}{\Leftrightarrow} \quad T = T^{\text{opt}} + T_Q^{\text{fluct}}(E)$$

$$T_q^{\text{fluct}}(E) = H_{Pd}\frac{1}{E - H_{dd} - W_{dd}} H_{dq} \frac{1}{E - H_{qq} - H_{qd}\dfrac{1}{E - H_{dd} - W_{dd}} H_{dq}} H_{qd} \frac{1}{E - H_{dd} - W_{dd}} H_{dP}$$

$$T_q^{\text{fluct}}(E) = \frac{1}{2\pi}\sum_q \frac{\gamma_{cq}(E)\gamma_{c'q}(E)}{E - \mathsf{E}_q(E)}, \qquad \gamma_{cq}(E) = \sum_d \frac{g_{cd}(E) g_{dq}(E)}{E - \mathsf{E}_d(E)}$$