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

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Energy structures in cross sections

**Fig. 6.** Photocapture of protons by $\text{Al}^{27}$ to the ground state of $\text{Si}^{28}$. The data is presented for various stages of resolution. From ref. 26.
Why KKM?

- A framework based on Feshbach’s projection operators
- Central result:
  - \[ T = T_{\text{background}} + T_{\text{resonant}} = T_{\text{average}} + T_{\text{fluctuating}} \]
- A foundation for derived statistical theories:
  - Kerman-McVoy
    - Designed for two step processes like \( A(d,p)B^*, B^* \rightarrow A+n \)
    - 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
HPC numerical simulation of formal theories of statistical nuclear reactions

- UNEDF SciDAC:
- www.unedf.org
Kawai-Kerman-McVoy:

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

\[ P \quad \text{PHQ} \quad Q \]

continuum

bound

compound
Feshbach’s projection operators

\[ H\Psi = E\Psi \]

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

\[
\begin{align*}
(E - H_{PP})P\Psi &= H_{PQ}\Psi \\
(E - H_{QQ})Q\Psi &= H_{QP}\Psi \\
(E - H_{PP})\chi &= 0
\end{align*}
\]

Two-potential formula yields

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

\[
\equiv T_{\text{background}} + T_{\text{resonant}}
\]
KKM subtraction

\[ (E - H_{PP})P\Psi = H_{PQ}\Psi \]
\[ (E - H_{QQ})Q\Psi = H_{QP}\Psi \]
\[ Q\Psi = \frac{1}{E - H_{QQ}} H_{QP}\Psi \]

\[ (E - H_{PP})P\Psi = H_{PQ} \frac{1}{E - H_{QQ}} H_{QP}P\Psi \]
\[ (E - H_{opt})P\Psi = 0 \]

\[ H_{opt} \equiv H_{PP} + H_{PQ} \frac{1}{E - H_{QQ} + iL} H_{QP} \]

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

\[ = H_{PQ} \sqrt{\frac{iL}{E - H_{QQ} + iL}} \frac{1}{E - H_{QQ}} \sqrt{\frac{iL}{E - H_{QQ} + iL}} H_{QP}P\Psi \]

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

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

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

Use \( H_{opt} \) to rewrite Eq. (3)
KKM Fluctuation T-matrix

\[
\begin{align*}
(E - H_{\text{opt}}) P \Psi &= V_{PQ} \Psi \\
(E - H_{\text{QQ}}) Q \Psi &= V_{QP} \Psi \\
(E - H_{\text{opt}}) P \Psi &= 0
\end{align*}
\]

Two-potential formula yields

\[
\Rightarrow T = \langle \phi | H_{\text{opt}} | \overline{\Psi} \rangle + \langle \overline{\Psi} | V_{PQ} \frac{1}{E - H_{\text{QQ}} - V_{QP} \frac{1}{E - H_{\text{opt}}} V_{QP}} | \overline{\Psi} \rangle
\]

\[
\equiv T_{\text{optical}} + T_{\text{fluctuation}}
\]

\[
\Rightarrow \langle T_{\text{fluctuation}} \rangle \approx 0
\]

is the central result of the KKM

\[
\Rightarrow \langle \sigma \rangle \approx \sigma_{\text{optical}} + \langle \sigma_{\text{fluctuation}} \rangle
\]
Expand T-matrix in eigenvalues/vectors:

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

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

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

\[ \sum_q | \tilde{q} \rangle \langle \tilde{q} | = 1 \]

\[ \sum_j | Q_j \rangle \langle Q_j | = 1 \]

\[ \langle \tilde{q} | \tilde{q}' \rangle = \delta_{\tilde{q}, \tilde{q}'} \]

\[ \langle Q_j | Q_j \rangle = \delta_{jj} \]

\[ T_{cc'} = T^{(0)}_{cc'} + \sum_{\tilde{q}} \langle \chi_c | H_{PQ} | \tilde{q} \rangle \frac{1}{E - \hat{\mathcal{E}}_q} \langle \tilde{q} | H_{QP} | \chi_{c'} \rangle \]

\[ T_{cc'} = T^{(0)}_{cc'} + \frac{1}{2\pi} \sum_{\tilde{q}} \frac{\hat{g}_{cq} \hat{g}_{c'q}}{E - \hat{\mathcal{E}}_q} \]

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

\[ \langle T_{cc'}^{\text{fluct}}(E) \rangle_I \equiv \frac{I}{2\pi} \int \frac{dE'}{(E - E')^2 + \frac{I^2}{4}} T_{cc'}^{\text{fluct}}(E') \]
### Preliminary Results:

<table>
<thead>
<tr>
<th>Eigenvalues/vectors</th>
<th>Average Ratio</th>
<th>SQRT(Variance)</th>
</tr>
</thead>
<tbody>
<tr>
<td>E-independent</td>
<td>0.0037</td>
<td>0.0053</td>
</tr>
<tr>
<td>E-dependent</td>
<td>0.0042</td>
<td>0.0049</td>
</tr>
</tbody>
</table>

**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
- \( E = 20 \text{ MeV} \)
- 100 \( E' \) points for Lorentzian averaging between 18 and 22 MeV
- Lorentzian averaging width \( I = 0.5 \text{ MeV} \)
- s-wave only
- Strongly overlapping resonances

**Histograms of \( |T_{\text{fluct}}|/|T_{opt}| \) for E-(in)dependent eigenvalues/vectors**
Test approximations in KKM derivation

- The E-dependence makes E-averaging more accurate

\[
T_{cc'} = \overline{T_{cc'}} + \frac{1}{2\pi} \sum_q g_{qc}(E)g_{qc'}(E) \left( \frac{E}{E - E_q(E)} \right) = \overline{T_{cc'}} + T_{cc'}^{\text{fluct}}
\]

\[
\Rightarrow \langle \sigma_{cc'}^{\text{fluct}} \rangle \sim \left( \left| T_{cc'}^{\text{fluct}} \right|^2 \right)_I
\]

\[
\mathbb{E} \left[ \sum_q \frac{g_{qc}g_{qc'}^{*} g_{qc}g_{qc'}^{*}}{E - E_q(E) E - E_q^{*}(E)} \right]_I
\]

\[
\mathbb{E} \left[ \frac{2\pi}{D_q \Gamma_q} \langle g_{qc}g_{qc'}^{*} g_{qc}g_{qc'}^{*} \rangle_q \right]
\]

\[
\mathbb{E} X_{cc} X_{c'c'} + X_{cc'} X_{c'c} \quad \text{where} \quad X_{cc'} \equiv \left( \frac{2\pi}{D\Gamma} \right)^{1/2} \langle g_{qc}g_{qc'}^{*} \rangle_q
\]

Random Phase Hypothesis

Preliminary results are analyzed.
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

\[
\langle \sigma_{cc'}^{\text{fl}} \rangle_I \sim X_{cc'}X_{c'c} + X_{cc'}X_{c'c}
\]

\[
X_{cc'} = \left\langle g_{cq}g_{c'q}^* \right\rangle_I
\]

\[
\langle \sigma_{cc'}^{\text{fl}} \rangle_I \sim \frac{1}{\sum P_{c''}} \left\{ P_{cc}P_{c'c'} + P_{cc'}P_{cc'} + \ldots \right\}
\]

\[
P_{cc'} = (1 - SS^*)_{cc'} = X_{cc'}Tr(X) + (X^2)_{cc'}
\]
Doorway states in the KKM theory

\[ P \quad PHQ \quad Q \]

continuum

\[ d \quad dHq \quad q \]

compound

\[ Q \quad bound \]
KKM extended to intermediate structure

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

\[ T = T^P + T^d + T^q(E) \]
\[ T = T^{\text{int}} + T_q^{\text{fluct}}(E) \]
\[ T = T^P + T^Q(E) \]
\[ T = T^{\text{opt}} + T_Q^{\text{fluct}}(E) \]

\[ T_q^{\text{fluct}}(E) = H_{pd} \frac{1}{E - H_{dd} - W_{dd}} H_{dq} \frac{1}{E - H_{qq} - H_{qd}} \frac{1}{E - H_{dd} - W_{dd}} H_{dp} \]

\[ T_q^{\text{fluct}}(E) = \frac{1}{2\pi} \sum_q \gamma_{cq}(E) \gamma_{c'q}(E) \]
\[ \gamma_{cq}(E) = \sum_d \frac{g_{cd}(E)g_{dq}(E)}{E - E_d(E)} \]
KKM extended to intermediate structure

\[ T = T^P + T^d + T^q(E) \]

\[ \langle T \rangle_{I_{\text{int}}} = T^P + T^d + \langle T^q(E) \rangle_{I_{\text{int}}} \]

\[ T^{\text{fluct}}_q(E) = T - \langle T \rangle_{I_{\text{int}}} = T^q(E) - \langle T^q(E) \rangle_{I_{\text{int}}} \]

\[ T^{\text{fluct}}_q(E) = \frac{1}{2\pi} \sum_q \frac{\gamma_{cq}(E)\gamma_{c'q}(E)}{E - E_q(E)} \]

\[ \gamma_{cq}(E) = \gamma_{cq}(E) \sqrt{\frac{iI_{\text{int}}}{E - E_q(E) + iI_{\text{int}}}} \]

\[ T = \langle T \rangle_{I_{\text{int}}} + T^{\text{fluct}}_q(E) \]

- Energy average over
  - “intermediate” structure
  - Finer than “gross”, but coarser than “fine” structure
KKM extended to intermediate structure

\[ T = \langle T \rangle_{I_{\text{int}}} + T_{q}^{\text{fluct}} (E) \]

\[ \langle T \rangle_{I_{\text{int}}} \approx T_{\text{int}} \]

\[ H_{\text{int}} = H_{pp} + H_{pd} \frac{1}{E - H_{dd} - H_{dq}} + \frac{1}{E - H_{qq} + iI_{\text{int}}} H_{qd} \]

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

\[ T = T_{\text{int}}^{\text{opt}} + T_{q}^{\text{fluct}} (E) \]

\[ \langle T_{q}^{\text{fluct}} (E) \rangle_{I_{\text{int}}} \approx 0 \]
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

<table>
<thead>
<tr>
<th>nq</th>
<th>Avg(T_kkm)/Avg(T)</th>
<th>Non-overlapping res.’s</th>
<th>Overlapping res.’s</th>
</tr>
</thead>
<tbody>
<tr>
<td>440</td>
<td>0.15</td>
<td></td>
<td>0.15</td>
</tr>
<tr>
<td>840</td>
<td>0.16</td>
<td></td>
<td>0.12</td>
</tr>
</tbody>
</table>
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
  • $E \sim E_1, E_2, ..., E_n$
  • instead of doing these in sequence, do them at once
    • form at most $n$ subcommunicators of size $P \times Q; (np \sim n \times P \times Q)$
    • $P, Q$ 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