Statistical Properties of Kawai-Kerman-McVoy T-matrix

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Abstract. Kawai, Kerman and McVoy (KKM) derived an optical background-plus-fluctuations representation of T-matrix, $T = T^{\rm opt} + T^{\rm fluct}$, so that an energy average of $T^{\rm fluct}$ over a single-particle resonance width is expected to be negligibly small (*Ann. of Phys.* **75**, 156 [1973]). We investigate this property numerically in a simple model with 1,600 compound nuclear levels and 40 channels, coupled via a random interaction. We find that the energy average of the fluctuating term is much smaller than the optical background, $T^{\rm opt}$, in support of the KKM result. A self-contained derivation of KKM T-matrix is presented.

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INTRODUCTION

Kawai, Kerman, and McVoy [1] transformed a conventional background-plus-resonant representation of T-matrix

$$T_{cc'}(E) = T^{(0)}_{cc'}(E) + \frac{1}{2\pi}\sum_q \frac{\hat{g}_{qc}(E)\hat{g}_{qc'}(E)}{E-\widehat{\mathscr{E}}_q(E)}, \qquad (1)$$

into a more convenient optical background-plus-fluctuations representation [1]

$$T_{cc'}(E) = T^{\rm opt}_{cc'}(E) + \frac{1}{2\pi}\sum_q \frac{g_{qc}(E)g_{qc'}(E)}{E-\mathscr{E}_q(E)}. \qquad (2)$$

where $\hat{g}_{qc}(E)$ are the partial-width amplitudes, and $\widehat{\mathscr{E}}_q(E)$ are the (complex) resonance energies, while $g_{qc}(E)$ and $\mathscr{E}_q(E)$ are their KKM equivalents[2]. Since $\langle T_{cc'}(E)\rangle_I \cong T^{\rm opt}_{cc'}(E)$ by definition, the energy average of the fluctuating term ought to be negligibly small, relative to $T^{\rm opt}_{cc'}(E)$:

$$\left\langle \sum_q \frac{g_{qc}(E)g_{qc'}(E)}{E-\mathscr{E}_q(E)} \right\rangle_I \ll T^{\rm opt}_{cc'}(E), \qquad (3)$$

where the energy averaging interval, I, is on the order of the width of a single particle resonance, ≈ 0.5 MeV. Due to this property, the cross terms that appear in computation of energy averaged cross section, average to zero, and the cross section separates into its optical and fluctuation contributions. This is not the case in the original representation in Eq. (1), because the energy average of the resonant term does not vanish.

Our numerical model resembles that of an earlier numerical study of KKM results [3] but with much larger statistical samples. In verifying Eq. (3) numerically we have ignored the energy dependence of $\mathscr{E}_q(E)$. The effect of the said energy dependence on energy averaged quantities will be studied in a later work. Studies of more elaborate statistical quantities appearing in KKM, or in a later elaboration [4], are also planned.

FORMAL DERIVATION

Derivation of Eqs. (1–2) follows the steps of Refs. [1], and [2], while spelling out the details needed for a numerical implementation. A formal Schrödinger equation

$$H\Psi = E\Psi \qquad (4)$$

along with Feshbach's [2] projection operators P and Q ($P+Q=1$) applied to Eq. (4) yields

$$(E-H_{PP})P\Psi = H_{PQ}Q\Psi, \qquad (5)$$
$$(E-H_{QQ})Q\Psi = H_{QP}P\Psi. \qquad (6)$$

Solving Eq. (5) for $P\Psi$ yields

$$P\Psi^{(+)} = P\chi^{(+)} + \frac{1}{E^{(+)}-H_{PP}}H_{PQ}Q\Psi, \qquad (7)$$

where χ is a homogenous solution of

$$(E-H_{PP})\chi = 0, \qquad (8)$$
$$H_{PP} = K_{PP} + V^{(0)}_{PP}. \qquad (9)$$

[1] In KKM the S-matrix was used, but we find T-matrix more convenient for derivation. The essential results of KKM are unaffected.
[2] For a more detailed definitions see [1].

K_{PP} is the kinetic energy. Inserting Eq. (7) into Eq. (5) and solving for $Q\Psi$ yields

$$Q\Psi = \frac{1}{E - H_{QQ} - W_{QQ}} H_{QP} P\chi^{(+)}. \tag{10}$$

where we defined

$$W_{QQ} \equiv H_{QP} \frac{1}{E^{(+)} - H_{PP}} H_{PQ} = H_{QP} G_P H_{PQ}. \tag{11}$$

We apply the two-potential formula to Eq. (5):

$$\begin{aligned} T &= T^{(0)} + T^{(1)} && (12)\\ &= \langle \phi^{(-)} | V_{PP}^{(0)} | \chi^{(+)} \rangle + \langle \chi^{(-)} | H_{PQ} | Q\Psi \rangle && (13) \end{aligned}$$

Inserting $Q\Psi$ into the expression for $T^{(1)}$ yields

$$T^{(1)} = \langle \chi^{(-)} | H_{PQ} \frac{1}{E - H_{QQ} - W_{QQ}} H_{QP} | \chi^{(+)} \rangle \tag{14}$$

A spectral decomposition of Eq. (14) is performed by a bi-orthogonal basis set $\{|\hat{q}\rangle, |\tilde{\hat{q}}\rangle\}$ of eigenfunctions of a complex symmetric operator $H_{QQ} + W_{QQ}$:

$$\begin{aligned} [H_{QQ} + W_{QQ}] |\hat{q}\rangle &= \widehat{\mathscr{E}}_q |\hat{q}\rangle, && (15)\\ \langle \tilde{\hat{q}}| [H_{QQ} + W_{QQ}] &= \langle \tilde{\hat{q}}| \widehat{\mathscr{E}}_q, && (16) \end{aligned}$$

where the slow energy dependence of eigenvalues, $\widehat{\mathscr{E}}_q = \widehat{E}_q - i\widehat{\Gamma}_q/2$, via $W_{QQ}(E)$, has been neglected in this work. Using the completeness and bi-orthogonality relations

$$1 = \sum_q |\hat{q}\rangle\langle\tilde{\hat{q}}|, \qquad \langle \tilde{\hat{q}} | \hat{q}' \rangle = \delta_{qq'} \tag{17}$$

in the expression for $T^{(1)}$, with explicit channel labels displayed, yields

$$T^{(1)}_{cc'}(E) = \frac{1}{2\pi} \sum_q \frac{\hat{g}_{cq}(E) \hat{g}_{c'q}(E)}{E - \widehat{\mathscr{E}}_q}, \tag{18}$$

where partial width amplitudes are

$$\hat{g}_{cq}(E) = \sqrt{2\pi} \langle \chi_c^{(-)}(E) | H_{PQ} | \hat{q} \rangle. \tag{19}$$

In the last step we took advantage of a symmetric property of $H_{QQ} + W_{QQ}$, which implies $\langle Q_j | \hat{q} \rangle = \langle \tilde{\hat{q}} | Q_j \rangle$ for any eigenvector $|Q_j\rangle$ of H_{QQ}, and consequently $\langle \tilde{\hat{q}} | H_{QP} | \chi^{(+)}_{c'} \rangle = \langle \chi^{(-)}_{c'} | H_{PQ} | \hat{q} \rangle$ for a Hermitean H. Inserting Eq. (18) into Eq. (12) yields Eq. (1).

To derive KKM separation of T-matrix into optical and fluctuating parts, stated in Eq. (2), a two-potential formula in Eq. (13) will be used, with the pair of potentials $(V_{PP}^{(0)}, H_{PQ})$ replaced by $(V_{PP}^{\rm opt}, V_{PQ})$, to be given in Eqs. (24) and (27), respectively. To derive a formal expression for $V_{PP}^{\rm opt}$, energy averaging will be performed. Lorentzian averaging is chosen because of a convenient analytical solution to averaging:

$$\langle F(E) \rangle_I = \frac{I}{\pi} \int dE' \frac{F(E')}{(E'-E)^2 + I^2} = F(E + iI), \tag{20}$$

where a contour integration in the upper half plane was performed, and it is assumed that function F has no poles in the upper half plane. Eliminating $Q\Psi$ from Eqs. (5–6) in favor of $P\Psi$ yields

$$[E - H_{PP} - H_{PQ} G_Q(E) H_{QP}] P\Psi = 0, \tag{21}$$

where $G_Q(E) \equiv \frac{1}{E - H_{QQ}}$. The Lorentzian averaging formula when applied to the T-matrix of the Schrödinger equation above yields:

$$[E - H_{PP} - H_{PQ} G_Q(E + iI) H_{QP}] \overline{P\Psi} = 0, \tag{22}$$

where $\overline{P\Psi}(E) \equiv \langle P\Psi(E) \rangle_I \cong P\Psi(E + iI)$ is the optical wavefunction. We define optical Hamiltonian

$$H_{PP}^{\rm opt} \equiv H_{PP} + H_{PQ} G_Q(E + iI) H_{QP}, \tag{23}$$

from which $V^{\rm opt}$ can be determined using Eq. (9) as

$$V_{PP}^{\rm opt} \equiv V_{PP}^{(0)} + H_{PQ} G_Q(E + iI) H_{QP}. \tag{24}$$

$H^{\rm opt}$ in Eq. (23) is used to rewrite Eq. (21) as

$$\left\{ E - H_{PP}^{\rm opt} - H_{PQ} [G_Q(E) - G_Q(E + iI)] H_{QP} \right\} P\Psi = 0 \tag{25}$$

Since $G_Q(E) - G_Q(E + iI) = iI G_Q(E) G_Q(E + iI)$, the above can be rewritten as:

$$\left[E - H_{PP}^{\rm opt} - V_{PQ} G_Q(E) V_{QP} \right] P\Psi = 0, \tag{26}$$

where

$$V_{PQ} = H_{PQ} \sqrt{iI G_Q(E + iI)} = H_{PQ} \sqrt{\frac{iI}{E - H_{QQ} + iI}}. \tag{27}$$

Eq. (26) is equivalent to two coupled equations, analogous to Eqs. (5–6):

$$\begin{aligned} \left(E - H_{PP}^{\rm opt} \right) P\Psi &= V_{PQ} Q\Psi, && (28)\\ (E - H_{QQ})\, Q\Psi &= V_{QP} P\Psi. && (29) \end{aligned}$$

This observation allows us to leverage the entire derivation leading to Eqs. (18–19), by making these direct substitutions:

$$H_{PP} \to H_{PP}^{\rm opt}, \;\; V_{PP}^{(0)} \to V_{PP}^{\rm opt}, \;\; H_{PQ} \to V_{PQ}, \;\; \chi \to \overline{\Psi}, \tag{30}$$

$$W_{QQ} \to W_{QQ}^{\rm opt} \equiv V_{QP} \frac{1}{E - H_{PP}^{\rm opt}} V_{PQ} = V_{QP} G_P^{\rm opt} V_{PQ}. \tag{31}$$

The above substituions necessiate that the bi-orthogonal basis $\{|\hat{q}\rangle, |\tilde{\hat{q}}\rangle\}$ be replaced by the basis formed by the eigenfunctions of $H_{QQ} + W_{QQ}^{\rm opt}$, namely, $\{|q\rangle, |\tilde{q}\rangle\}$ with eigenvalues $\mathscr{E}_q = E_q - i\Gamma_q/2$. Putting all of this together yields [3]:

$$T_{cc'}(E) = T_{cc'}^{\rm opt}(E) + \frac{1}{2\pi}\sum_q \frac{g_{qc}(E) g_{qc'}(E)}{E - \mathscr{E}_q}, \qquad (32)$$

where KKM partial-width amplitudes are

$$g_{cq}(E) = \sqrt{2\pi}\langle \overline{\Psi}_c^{(-)}(E)|V_{PQ}(E)|q\rangle. \qquad (33)$$

NUMERICAL METHOD

First, we define projection operators P and Q :

$$P = \sum_c^{N_c}\int_r |r;c\rangle\langle r;c| \equiv 1 - Q, \qquad (34)$$

$$Q = \sum_j^{N_Q} |Q_j\rangle\langle Q_j|, \quad H_{QQ}|Q_j\rangle = E_j^{(Q)}|Q_j\rangle, \qquad (35)$$

where a shorthand notation $\int_r \equiv \int r^2 dr$ was used. P is in a spatial representation, as in Ref. [5], and the normalization of $|r;c\rangle$ ensures that $P^2 = P$. $\{|Q_j\rangle\}$ consists of N_Q equidistant levels [4]. Their energies, $E_j^{(Q)}$, are input parameters to numerical computation chosen to cover the averaging energy region around the total energy E. The number of levels N_Q, the number of channels N_c, their threshold energies, E_c, and number of interaction points N_R are all model parameters. With these definitions we are able to evaluate $\hat{g}_{cq}$ in Eq. (19)

$$\hat{g}_{cq}(E) = \sqrt{2\pi}\sum_{c'}^{N_c}\sum_j^{N_Q}\int_r \langle \chi_c^{(-)}(E)|r;c'\rangle\langle r;c'|H|Q_j\rangle\langle Q_j|\hat{q}\rangle. \qquad (36)$$

(Note that $\chi_{cc'}^{(-)}(E;r) \equiv \langle \chi_c^{(-)}(E)|r;c'\rangle$.) The coupling between P and Q spaces is modeled numerically via $\langle r;c|H|Q_j\rangle$

$$H_{cj}(r) \equiv \langle r;c|H|Q_j\rangle = \sum_k^{N_R} h_{cjk}\frac{\delta(r - r_k)}{r r_k}, \qquad (37)$$

where h_{cjk} are real random numbers taken from a Gaussian distribution with a zero mean [6], and the $\{r_k\}$ are chosen as N_R equidistant radial points in the nuclear interior. The width of the Gaussian distribution controls the strength of the coupling between P and Q spaces, and since the coupling gives widths to the resonances, a degree of overlapping among resonances. The results presented are relevant in the overlapping resonance regime. Resonance energies and widths are given by the eigenvalues $\widehat{\mathscr{E}}_q = \widehat{E}_q - i\widehat{\Gamma}_q/2$ of operator $(H_{QQ} + W_{QQ})$, which in $\{|Q_j\rangle\}$ basis reads:

$$\langle Q_j|H_{QQ} + W_{QQ}|Q_k\rangle = E_j^{(Q)}\delta_{jk} + W_{jk}(E), \qquad (38)$$

where $W_{jk}(E)$ is found by inserting Eqs. (34) and (37) into (11):

$$W_{jk}(E) = \sum_{cc'}^{N_c}\int_r\int_{r'}\langle Q_j|H|r;c\rangle\langle r;c|G|r';c'\rangle\langle r';c'|H|Q_k\rangle,$$
$$= \sum_{cc'}^{N_c}\sum_{ll'}^{N_R} h_{cjl}G_{cc'}(E;r_l,r_{l'})h_{c'kl'}, \qquad (39)$$

where $G_{cc'}(E;r,r') \equiv \langle r;c|G|r';c'\rangle$. For simplicity, $V_{PP}^{(0)}$ was set to zero, so that $T^{(0)} = 0$, χ is a free particle wave function, and $G_{cc'}(E;r,r')$ is a free-particle Green function. For simplicity, we consider s-wave channel only, for which $\chi = j_0$, a zero-order Bessel function, and

$$G_{cc'}(E;r,r') = -\frac{k_c^3\delta_{cc'}}{E - E_c}\left[\frac{\sin(k_c r_<)}{k_c r_<}\frac{\exp(ik_c r_>)}{k_c r_>}\right], \qquad (40)$$

where $r_<$ ($r_>$) is the smaller (larger) of $\{r,r'\}$, and $k_c = \sqrt{2m(E - E_c)}/\hbar$, where E_c is a threshold of channel c. The eigenvalues and eigenvectors [5] of $(H_{QQ} + W_{QQ})$ are computed by ZGEEV subroutine of Lapack library [7]:

$$|\hat{q}\rangle = \sum_j \widehat{C}_{jq}|Q_j\rangle \equiv \sum_j |Q_j\rangle\langle Q_j|\hat{q}\rangle \qquad (41)$$

by returning coefficients $\widehat{C}_{jq}$. Inserting Eqs. (37) and (41) into (36) gives

$$\hat{g}_{cq}(E) = \sqrt{2\pi}\sum_j \widehat{H}_{cj}(E)\widehat{C}_{jq}, \qquad (42)$$

where

$$\widehat{H}_{cj}(E) \equiv \sum_{c'}\int_r \chi_{cc'}^{(-)}(E;r)H_{c'j}(r), \qquad (43)$$

for an s-wave free particle $\widehat{H}_{cj}(E) \to \sum_k j_0(k_c r_k)h_{cjk}$. All quantities needed to model Eq. (1) have thus been expressed in terms of input parameters.

Next we express quantites entering Eq. (2) in terms of the same input parameters. The optical wave function $\overline{P\Psi}$ is obtained by Lorentzian averaging of Eq. (7):

$$\overline{P\Psi} = \chi + \frac{1}{E^{(+)} - H_{PP}}H_{PQ}\frac{1}{E - H_{QQ} - W_{QQ} + iI}H_{QP}\chi, \qquad (44)$$

[3] We neglect the energy dependance of $\mathscr{E}_q$, as was done in Eq. (18).
[4] Wigner distribution will be considered in a later work.
[5] The energy dependence of eigenvectors $\widehat{C}_{jq}$ is neglected; these are computed once at E and used throughout the averaging interval.

where it is assumed that $1/(E-H_{PP})$ does not vary appreciably over the averaging interval. The same method yields the optical Green's function:

$$G_P^{\rm opt} = G_P + G_P H_{PQ} \frac{1}{E - H_{QQ} - W_{QQ} + iI} H_{QP} G_P. \quad (45)$$

We can now express $W_{jk}^{\rm opt} \equiv \langle Q_j | V_{QP} G^{\rm opt} V_{PQ} | Q_k \rangle$ as

$$W_{jk}^{\rm opt}(E) = \sqrt{\frac{iI}{E - E_j^{(Q)} + iI}} \sqrt{\frac{iI}{E - E_k^{(Q)} + iI}} \times \left\{ W_{jk} + \sum_{qj'k'} W_{jj'} \widehat{C}_{j'q} \frac{1}{E - \widehat{\mathscr{E}}_q + iI} \widehat{C}_{k'q} W_{k'k} \right\} \quad (46)$$

and then solve for eigenvectors of $(E_j^{(Q)}\delta_{jk} + W_{jk}^{\rm opt})$, as in Eq. (41),

$$|q\rangle = \sum_j C_{jq} |Q_j\rangle. \quad (47)$$

Similarly, Eq. (44) is used to write Eq. (33) as

$$g_{cq}(E) = \sqrt{2\pi} \sum_j C_{jq} \widehat{V}_{cj}(E), \quad (48)$$

where

$$\widehat{V}_{cj}(E) = \sqrt{\frac{iI}{E - E_j^{(Q)} + iI}} \times \left\{ \widehat{H}_{cj} + \sum_{kj'q} \widehat{H}_{cj'} \widehat{C}_{j'q} \frac{1}{E - \widehat{\mathscr{E}}_q + iI} \widehat{C}_{kq} W_{kj} \right\}. \quad (49)$$

Note that W_{jk} and $\widehat{C}_{jq}$ above are those given in Eqs. (39) and (41), respectively; hence, these matrices are computed only once. This ensures a self-consistent computation of optical and non optical quantities.

RESULTS

The model parameters listed below were chosen to mimic the overlapping resonance regime. The energy density of Q-levels is a key parameter influencing the accuracy of the computation of Eq. (3). The largest run contained $N_Q = 1{,}600$ equidistant levels spanning 10 – 30 MeV, sufficient for a strong overlap $\langle\Gamma\rangle/\langle D\rangle = 23.5$.

$T_{cc'}^{\rm fluct}$ was energy averaged with a Lorentzian weight around the total energy $E = 20$ MeV, and a half-width [6] $I = 0.25$ MeV. The Lorentzian energy average was performed over 100 equidistant points between 18 and 22 MeV for each pair of channel indices (c,c'), where $c = 1,2,\ldots,N_c$; $N_c = 40$ channels, and $E_c = (c-1)\times 0.1$ MeV. The random interaction, h_{cjk}, was defined on $N_R = 20$ equidistant radial points between the origin and 7 fm. The coupling strength was set to $\langle h_{cjk}^2\rangle^{1/2} = 0.5$ MeV fm$^{3/2}$. For simplicity, we set $V_{PP}^{(0)} = 0$, so that $T_{cc'}^{\rm opt}$ could be computed as $T_{cc'}^{\rm opt} \cong \langle T_{cc'}^{(1)}\rangle_I$. For s-wave resonances, the average of $\langle T_{cc'}^{\rm fluct}\rangle_I / T_{cc'}^{\rm opt}$ over all channels was found to be 0.0024 with a standard deviation of 0.0037 (see Fig. 1) in support of the KKM result in Eq. (3).

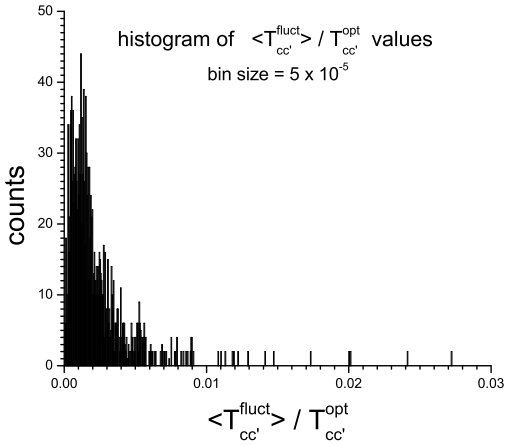

FIGURE 1. Histogram of $\langle T_{cc'}^{\rm fluct}\rangle_I / T_{cc'}^{\rm opt}$ for 40×40 channel pairs. The average value of the ratio is 0.0025 with a standard deviation of 0.0037. $\langle\Gamma\rangle/\langle D\rangle = 23.5$ in the averaging region.

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[6] Note that I, as used in Eq. (20), corresponds to one half of the FWHM of the Lorentzian. Hence, $I = 0.25$ MeV amounts to an averaging interval of 0.5 MeV, tantamount to a single particle resonance width.