ON THE NON-INVARIANCE OF DISTRIBUTIONS OF REACTION MATRIX PARAMETERS UNDER CHANGES IN BOUNDARY CONDITIONS

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Abstract

Contrary to current opinion, the statistical distributions of level spacings and reduced widths when applied to the reaction matrix are not invariant under changes in the boundary condition matrix or the matching radius. General arguments are given, together with specific examples which violate the invariance requirements. We conclude that it may be the parameters of the collision matrix which should be analysed and considered as the invariant parameters. It is shown that if, for a specific set of boundary conditions, the distributions of level spacings and reduced widths are uncorrelated, then correlations between the level spacings and widths must exist when different boundary conditions are used.

I. Introduction

The parameters which occur in statistical theories of nuclear reactions usually depend on the statistical properties of the parameters in the reaction matrix **R**, and for this reason the statistics of R-matrix parameters have been widely investigated (Lynn 1968). Distribution laws for level spacings and reduced widths have been derived by Wigner (1956) and Porter and Thomas (1956) respectively. Though no formal proof has ever been given, it is usually assumed that the statistical distributions of R-matrix parameters are independent of the boundary conditions used in the definition of the R-matrix. Lane and Thomas (1958) claimed this on physical grounds and supported their view with a plausibility argument. Teichmann and Wigner (1952), by considering the effect of changes in the boundary conditions, suggested the existence of correlations between the level spacings and the reduced widths. On the other hand, Lane and Thomas dismiss this argument as being based on mere speculation.

More recently, Moldauer (1964) investigated some of the statistical properties of the R-matrix numerically and concluded that they were not independent of the boundary conditions. He discovered that by fixing the distributions of the reaction matrix parameters and varying the boundary conditions, the distributions of parameters of the collision matrix varied; this should not occur. Unfortunately, changes in statistical distributions due to changes in boundary conditions are not investigated easily by computer experiments. The main difficulty is the restriction to a finite number of levels. Initially, an R-matrix may be constructed such that the distributions of the level spacings and reduced widths are independent of the sampling range. However, after changing the boundary conditions the resulting R-matrix no longer has this property. Distributions obtained by sampling the poles near the extremities

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of the range are generally different from those obtained by sampling near the centre of the range.

In this paper, the problem of whether or not the reaction matrix parameters vary with boundary conditions is investigated analytically for a single channel R-matrix by considering the moment-generating functions of the distributions. The statistics of R-matrix parameters are generally not invariant under changes in boundary conditions. This is demonstrated by considering first- and second-order variations in the moments and distributions due to variations in boundary conditions. It is shown that if there exists a special set of boundary conditions in which the level spacings and reduced widths are uncorrelated, then generally for other boundary conditions there must be correlations between the level spacings and reduced widths. Therefore the method of statistically sampling reaction matrix parameters from uncorrelated distributions in order to generate cross sections may only be valid for a particular set of boundary conditions.

II. Formulation of the Problem

In the Wigner and Eisenbud (1947) R-matrix formalism, the single channel scattering matrix is expressed in terms of the R-function

$$R(E) = \sum_{\lambda} \gamma_\lambda^2/(E_\lambda - E) + R_\infty\,, \tag{1}$$

where the γ_λ^2 are the reduced widths, the E_λ are the resonance poles, and R_∞ is a residual constant. The eigenvalues E_λ of the nuclear Hamiltonian are defined by imposing on the eigenfunctions, at a chosen radius a, boundary conditions which are characterized by a real constant B, as

$$[\mathrm{d}\psi_\lambda(r)/\mathrm{d}r]_{r=a} = (B/a)\psi_\lambda(a)\,, \tag{2}$$

where the $\psi_\lambda(r)$ are eigenfunctions, corresponding to the eigenvalues E_λ, of the nuclear Hamiltonian with the boundary conditions (2). The reduced width amplitudes are defined as

$$\gamma_\lambda^2 = (\hbar^2/2Ma)\psi_\lambda^2(a)\,, \tag{3}$$

where M is the reduced mass of the system.

If R_0 is an R-function corresponding to the boundary condition B_0 then the R-function for a different boundary condition B is given by the relation (Lane and Thomas 1958)

$$R = R_0\{1-(B-B_0)R_0\}^{-1}\,. \tag{4}$$

The collision function $\mathscr{S}$ is given by

$$\mathscr{S} = \Omega^2\{1-(L-B)R\}^{-1}\{1-(L^*-B)R\}\,, \tag{5}$$

where $\Omega = \exp(\mathrm{i}\phi)$, ϕ being the hard sphere phase shift, and $L = S+\mathrm{i}P$, S being the level shift and P the penetration factor. The function (5) is invariant under the transformation (4). It should also be invariant with respect to changes in the arbitrarily chosen radius a. We can express these invariances in the equations

$$\partial\mathscr{S}/\partial B = 0\,, \qquad \partial\mathscr{S}/\partial a = 0\,. \tag{6a, b}$$

The positions E'_λ of the poles in R are given by the solutions of the equation

$$1-(B-B_0)R_0 = 0 \tag{7}$$

and the residues are

$$\gamma_\lambda^2 = [(B-B_0)^2\mathrm{d}R/\mathrm{d}E]^{-1}_{E=E'_\lambda}\,. \tag{8}$$

Equation (4) was shown by Teichmann (1950) to be equivalent to the differential form

$$\partial R/\partial B = R^2\,. \tag{9}$$

By equating residues at the poles on either side of equation (9) we find

$$\frac{\partial E_\lambda}{\partial B} = -\gamma_\lambda^2\,, \qquad \frac{\partial \gamma_\lambda^2}{\partial B} = 2\gamma_\lambda^2 \sum_{\mu\neq\lambda} \frac{\gamma_\mu^2}{E_\mu - E_\lambda}\,. \tag{10a, b}$$

These relations also follow from equations (6a) and (5).

In order to study the statistics of R-matrix parameters, Wigner (1956) introduced the concept of the statistical R-function in which the reduced widths γ_λ^2 and level spacings D_λ, given by

$$D_\lambda = E_{\lambda+1} - E_\lambda\,, \tag{11}$$

have definite distributions which are independent of the sampling range. We shall consider the statistical R-function defined by equation (1) in which the summation over λ extends from $-\infty$ to $+\infty$. We suppose that there is some prescribed order in which positive and negative terms in equation (1) are to be summed.

The effects of changes in the boundary conditions on the statistics of the parameters is most conveniently investigated by means of moment-generating functions. The moment-generating function (Cramèr 1946) of a distribution $P(x)$ is the Laplace transform

$$\bar{P}(s) = \int_0^\infty \exp(-sx)\,P(x)\,\mathrm{d}x\,, \tag{12}$$

so that when $\bar{P}(s)$ is expanded in ascending powers of s

$$\bar{P}(s) = \sum_{k=0}^{\infty} \{(-1)^k/k!\}M_k s^k\,, \tag{13}$$

where M_k is the kth moment of the distribution. If the series (13) is absolutely convergent for some $s > 0$, the distribution is uniquely determined by its moments. Therefore the dependence of the distributions of level spacings and widths on the boundary conditions is completely determined by the dependence of the moments upon B and a.

Two common examples of the above which are used in calculations are as follows.

Wigner Distribution of Level Spacings

In this case

$$P(D)\,\mathrm{d}D = (\pi D/2\bar{D}^2)\exp\{-\pi D^2/(4\bar{D})^2\} \tag{14}$$

and

$$\bar{P}_D(s) = 1-\bar{D}s\exp\{(\bar{D}^2s^2)/\pi\}\operatorname{erfc}(\bar{D}s/\pi^{\frac{1}{2}}), \tag{15}$$

where

$$\operatorname{erfc}(x) = (2/\pi^{\frac{1}{2}})\int_x^\infty \exp(-t^2)\,\mathrm{d}t.$$

The Taylor expansion of (15) gives all of the moments of the distribution in terms of $\bar{D}$ alone:

$$\bar{P}_D(s) \approx 1-\bar{D}s+(2/\pi)\bar{D}^2s^2+\ldots \tag{16a}$$

and thus

$$M_0(D) = 1, \qquad M_1(D) = \bar{D}, \qquad M_2(D) = 4\bar{D}^2/\pi. \tag{16b}$$

Porter–Thomas Distribution of Reduced Widths

Here

$$P(\gamma^2)\,\mathrm{d}\gamma^2 = (2\gamma^2\pi\langle\gamma^2\rangle)^{-\frac{1}{2}}\exp(-\gamma^2/2\langle\gamma^2\rangle)\,\mathrm{d}\gamma^2 \tag{17}$$

and

$$\bar{P}_\gamma(s) = (1+2s\langle\gamma^2\rangle)^{-\frac{1}{2}} = 1-\langle\gamma^2\rangle s+\tfrac{3}{2}\langle\gamma^2\rangle^2s^2\ldots, \tag{18}$$

which yields

$$M_0(\gamma^2) = 1, \qquad M_1(\gamma^2) = \langle\gamma^2\rangle, \qquad M_2(\gamma^2) = 3\langle\gamma^2\rangle^2. \tag{19}$$

III. Level Spacing Distribution

Suppose when $B = B_0$ that D_λ and γ_λ^2 are uncorrelated. The dependence of the level spacings on B is obtained from equation (10a) as

$$\partial D_\lambda/\partial B = \gamma_\lambda^2-\gamma_{\lambda+1}^2. \tag{20}$$

Using the fact that

$$\partial D_\lambda/\partial B = \partial\langle D\rangle/\partial B, \tag{21}$$

where the angle brackets denote the average over λ, we find

$$\langle\partial\langle D\rangle/\partial B\rangle = \langle\gamma_\lambda^2-\gamma_{\lambda+1}^2\rangle = \langle\gamma^2\rangle-\langle\gamma^2\rangle = 0. \tag{22}$$

Similarly, by repeated differentiation of (22) we can show that for all n

$$\frac{\partial^n\langle D\rangle}{\partial B^n} = \left\langle\frac{\partial^{n-1}\gamma_\lambda^2}{\partial B^{n-1}}-\frac{\partial^{n-1}\gamma_{\lambda+1}^2}{\partial B^{n-1}}\right\rangle = 0. \tag{23}$$

This result reflects the well-known fact that the average density of levels is independent of B (Lane and Thomas 1958); however, it is not necessarily independent of a. Furthermore, we can show that the first derivatives of all higher moments vanish. Thus

$$\langle\partial D_\lambda^n/\partial B\rangle = \langle nD_\lambda^{n-1}(\gamma_\lambda^2-\gamma_{\lambda+1}^2)\rangle = n\langle D_\lambda^{n-1}\rangle\langle\gamma_\lambda^2-\gamma_{\lambda+1}^2\rangle = 0, \tag{24}$$

since D_λ and γ_λ^2 are uncorrelated.

Needless to say, if the moments are to be truly independent of B then all higher derivatives of all moments must be identically zero, that is,

$$\partial^n M_k / \partial B^n = 0 \qquad \text{for all} \quad (n, k)\,. \tag{25}$$

This is certainly not the case in general, as can be seen by considering the second derivative of the second moment $M_2(D)$.

From

$$\frac{\partial^2 D_\lambda^2}{\partial B^2} = 2(\gamma_\lambda^2 - \gamma_{\lambda+1}^2)^2 + 2D_\lambda\left(\frac{\partial \gamma_\lambda^2}{\partial B} - \frac{\partial \gamma_{\lambda+1}^2}{\partial B}\right) \tag{26}$$

we obtain

$$\frac{\partial^2 M_2}{\partial B^2} = \frac{\partial^2 \langle D^2 \rangle}{\partial B^2} = 2\langle(\gamma_\lambda^2 - \gamma_{\lambda+1}^2)^2\rangle + 2\left\langle D_\lambda\left(\frac{\partial \gamma_\lambda^2}{\partial B} - \frac{\partial \gamma_{\lambda+1}^2}{\partial B}\right)\right\rangle. \tag{27}$$

The first term on the right in equation (27) is nonzero and its value depends only on the distribution of the reduced widths. In general the second term will not cancel the first term as its value depends not only on the distribution of widths but also on the distribution of level spacings. The value of the second term can be determined. Using the fact that at B_0 widths and spacings are uncorrelated, we obtain from equation (10b)

$$\left\langle D_\lambda \frac{\partial \gamma_\lambda^2}{\partial B} \right\rangle = \langle \gamma^2 \rangle^2 \left\langle D_\lambda \sum_{\mu \neq \lambda} \frac{1}{E_\mu - E_\lambda} \right\rangle. \tag{28}$$

For those terms in equation (28) for which $\mu = \lambda - k$ $(k > 0)$, we have

$$\left\langle \frac{D_\lambda}{E_{\lambda-k} - E_\lambda} \right\rangle = -\left\langle D_\lambda \left(\sum_{i=1}^{k} D_{\lambda-i}\right)^{-1} \right\rangle = -\langle D \rangle \left\langle \left(\sum_{i=1}^{k} D_{\lambda-i}\right)^{-1} \right\rangle. \tag{29}$$

Writing

$$\left(\sum_{i=1}^{k} D_{\lambda-i}\right)^{-1} = \int_0^\infty \left(\prod_{i=1}^{k} \exp(-D_{\lambda-i}\, s)\right) \mathrm{d}s\,, \tag{30}$$

we find

$$\left\langle \frac{D_\lambda}{E_{\lambda-k} - E_\lambda} \right\rangle = -\langle D \rangle \int_0^\infty [\bar{P}_D(s)]^k \,\mathrm{d}s\,, \tag{31}$$

where $\bar{P}_D(s)$ is the moment-generating function of the distribution of level spacings. Similarly, those terms in equation (28) which have $\mu = \lambda + k$ $(k > 0)$ can be written as

$$\left\langle \frac{D_\lambda}{E_{\lambda+k} - E_\lambda} \right\rangle = \left\langle D_\lambda \left(\sum_{i=0}^{k-1} D_{\lambda+i}\right)^{-1} \right\rangle = k^{-1}, \tag{32}$$

which may also be expressed in integral form as

$$\left\langle \frac{D_\lambda}{E_{\lambda+k} - E_\lambda} \right\rangle = \langle D \rangle \int_0^\infty \exp(-k\langle D \rangle s)\,\mathrm{d}s\,. \tag{33}$$

Therefore, combining the relations (31) and (33), equation (28) becomes

$$\left\langle D_\lambda \frac{\partial \gamma_\lambda^2}{\partial B} \right\rangle = \langle \gamma^2 \rangle^2 \langle D \rangle \left(\sum_{k=1}^{\infty} \int_0^\infty \{\exp(-k\langle D \rangle s) - [\bar{P}_D(s)]^k\}\right) \mathrm{d}s\,. \tag{34}$$

The two summations in (34) must of course be carried out simultaneously in the same order as used to define the summation in equation (1). To avoid difficulties arising from the lower limits of the integrations, we replace them by a small positive ϵ and consider the limit as ϵ tends to zero. Since for all $s > \epsilon$ the two series in equation (34) are absolutely convergent, the summations may be taken inside the integrals. Summing the series separately we obtain when $\epsilon \to 0$

$$\left\langle D_\lambda \frac{\partial \gamma_\lambda^2}{\partial B} \right\rangle = \langle \gamma^2 \rangle^2 \langle D \rangle \int_0^\infty \left(\frac{\exp(-\langle D \rangle s)}{1-\exp(-\langle D \rangle s)} - \frac{\bar{P}_D(s)}{1-\bar{P}_D(s)} \right) \mathrm{d}s \,. \tag{35}$$

In terms of averages we obtain finally

$$\partial^2 \langle D^2 \rangle / \partial B^2 = 4(\langle \gamma^4 \rangle - \langle \gamma^2 \rangle^2) + 4\langle \gamma^2 \rangle^2 C(\langle D \rangle) \,, \tag{36}$$

where

$$C(\langle D \rangle) = \langle D \rangle \int_0^\infty \left(\frac{\exp(-\langle D \rangle s)}{1-\exp(-\langle D \rangle s)} - \frac{\bar{P}_D(s)}{1-\bar{P}_D(s)} \right) \mathrm{d}s \,. \tag{37}$$

We note that the integral on the right of (37) exists only if $\bar{P}_D(s)$ tends to zero faster than s^{-1} as s tends to infinity. For large s, we may write

$$\begin{aligned} \bar{P}_D(s) &= \int_0^\infty \exp(-sD)\{P(0) + D(\mathrm{d}P/\mathrm{d}D)_{D=0} + \ldots\} \, \mathrm{d}D \\ &= s^{-1} P(0) + s^{-2} (\mathrm{d}P/\mathrm{d}D)_{D=0} + \ldots \,. \end{aligned} \tag{38}$$

Therefore, the above analysis holds only if

$$\lim_{D \to 0} P(D) = 0 \,, \tag{39}$$

which is an expression of the fact that levels repel each other. We note that often $\bar{P}_D(s)$ has the form $\bar{P}_D(\langle D \rangle s)$ and therefore that

$$C(\langle D \rangle) = \int_0^\infty \left(\frac{\exp(-u)}{1-\exp(-u)} - \frac{\bar{P}_D(u)}{1-\bar{P}_D(u)} \right) \mathrm{d}u \,, \tag{40}$$

which is independent of $\langle D \rangle$, and is therefore constant. Similarly, if $P(\gamma^2)$ can be written as a function $P(\gamma^2/\langle \gamma^2 \rangle)$ then $\bar{P}_\gamma(s)$ has the form $\bar{P}_\gamma(\langle \gamma^2 \rangle s)$ and the second moment of the distribution is a constant times $\langle \gamma^2 \rangle$. It follows that

$$\partial^2 \langle D^2 \rangle / \partial B^2 = \text{const.} \langle \gamma^2 \rangle^2 \,. \tag{41}$$

As an example, if we take the Wigner distribution of level spacings (14) and the Porter–Thomas distribution of reduced widths (17), we obtain

$$\partial^2 \langle D^2 \rangle / \partial B^2 = (8 - 4C) \langle \gamma^2 \rangle^2 \,, \tag{42}$$

where

$$\begin{aligned} C &= \int_0^\infty \left(\frac{1}{1-\bar{P}_D(u)} - \frac{1}{1-\exp(-u)} \right) \mathrm{d}u \\ &= \int_0^\infty \left(\frac{\exp(-u^2/\pi)}{u \operatorname{erfc}(u/\pi^{\frac{1}{2}})} - \frac{1}{1-\exp(-u)} \right) \mathrm{d}u \sim 0 \cdot 49 \,. \end{aligned} \tag{43}$$

IV. Distribution of Reduced Widths

If we consider equations (7) and (8), then since $R_0'(E_\lambda')$ is finite for every $B \neq B_0$, it follows that all γ_λ^2 tend to zero when $B - B_0$ tends to infinity. Thus the average reduced width $\langle\gamma^2\rangle$ is certainly not independent of B. We therefore examine the effect of the transformation (4) on the distribution of the quantities $\gamma_\lambda^2/\langle\gamma^2\rangle$. It is not difficult to see from equation (10b) that

$$\partial\langle\gamma^2\rangle/\partial B = 0\,, \tag{44}$$

though in general higher derivatives do not vanish. Using the fact that γ_λ^2 and D are uncorrelated, we obtain for $n > 1$

$$\frac{\partial^2}{\partial B^2}\left\langle\left(\frac{\gamma_\lambda^2}{\langle\gamma^2\rangle}\right)^n\right\rangle = 4n(n-1)\frac{\langle\gamma^{2n}\rangle\langle\gamma^2\rangle^2}{\langle\gamma^2\rangle^n}A + \left(2n(2n-1)\frac{\langle\gamma^{2n}\rangle\langle\gamma^4\rangle}{\langle\gamma^2\rangle^n} - 2n\frac{\langle\gamma^{2n+2}\rangle\langle\gamma^2\rangle}{\langle\gamma^2\rangle^n}\right)F\,, \tag{45}$$

where

$$A = \left\langle\sum_{\mu\neq\lambda}\sum_{\nu\neq\mu}(E_\mu - E_\lambda)^{-1}(E_\nu - E_\lambda)^{-1}\right\rangle, \qquad F = \left\langle\sum_{\mu\neq\lambda}(E_\mu - E_\lambda)^{-2}\right\rangle.$$

The conditions on A and F under which the second derivatives of all moments vanish can be represented by the set of simultaneous equations

$$a_n A + f_n F = 0\,, \qquad n = 2, 3, 4, \ldots, \tag{46}$$

where a_n and f_n are the coefficients in equation (45). Since F is always nonzero, the equations (46) can only be satisfied if:

(i) $A = 0$ and $f_n = 0$ for all n, and

(ii) a_n/f_n is a constant that is independent of n.

Clearly neither of these conditions is satisfied in general, and therefore the distribution of reduced widths must change when the value of B is altered.

V. Level Spacing Distribution after Small Change in Boundary Conditions

In Section III it was shown how the moments of the distribution of level spacings vary under small changes in B. However, from these results it is not easy to derive the corresponding change in the distribution function itself. The effect of a small change in the value of B on the shape of the distribution function can be calculated more easily by considering transformations between random variables.

Suppose that initially we have a set of level spacings $D_1, D_2, \ldots, D_N$ and a set of reduced widths $Y_1, Y_2, \ldots, Y_N$ such that the probability that D_i has a value between D and $D + \mathrm{d}D$ is $P(D)\,\mathrm{d}D$ and the probability that Y_i has a value between Y and $Y + \mathrm{d}Y$ is $Q(Y)\,\mathrm{d}Y$. Let us consider the effect of the transformation (4) on a particular D_λ, say D_1. We write the transformed level spacing as

$$\mathscr{D}_1 = f(D_1, \ldots, D_N;\ Y_1, \ldots, Y_N)\,. \tag{47}$$

The inverse transformation may be written as

$$D_1 = F(\mathscr{D}_1, D_2, ..., D_N;\ Y_1, Y_2, ..., Y_N). \tag{48}$$

Then the probability that $\mathscr{D}_1$ has a value between $\mathscr{D}$ and $\mathscr{D}+\mathrm{d}\mathscr{D}$ is given by $\mathscr{P}(\mathscr{D})\,\mathrm{d}\mathscr{D}$ where

$$\mathscr{P}(\mathscr{D}) = \int ... \int P\{F(\mathscr{D}, D_2, ..., D_N;\ Y_1, ..., Y_N)\}\{P(D_2)\,...\,P(D_N)\} \times\{Q(Y_1)\,...\,Q(Y_N)\}(\partial F/\partial\mathscr{D})\,\mathrm{d}D_2\,...\,\mathrm{d}D_N\,\mathrm{d}Y_1\,...\,\mathrm{d}Y_N. \tag{49}$$

This can be written as

$$\mathscr{P}(\mathscr{D}) = \langle P\{F(\mathscr{D}, D_2, ..., D_N;\ Y_1, ..., Y_N)\}\partial F/\partial\mathscr{D}\rangle, \tag{50}$$

where the average is taken over all variables except $\mathscr{D}$.

In particular, when $B = B_0+\delta B$ we can write to second order in δB

$$\mathscr{D}_i = D_i+(\gamma_i^2-\gamma_{i+1}^2)\delta B+\left(\gamma_i^2\sum_{\mu\neq i}\frac{\gamma_\mu^2}{E_\mu-E_i}-\gamma_{i+1}^2\sum_{\mu\neq i+1}\frac{\gamma_\mu^2}{E_\mu-E_{i+1}}\right)(\delta B)^2. \tag{51}$$

Using the same argument as that used to derive equations (31) and (33) we can obtain the inverse tranformation in order $(\delta B)^2$ as

$$\begin{aligned}
&F(\mathscr{D}, D_2, ..., D_N;\ \gamma_1^2, ..., \gamma_N^2)\\
&= \mathscr{D}-(\gamma_i^2-\gamma_{i+1}^2)\delta B-\left[\gamma_i^2\left\{\sum_{\mu>i}\gamma_\mu^2\left(\mathscr{D}+\sum_k D_{i+k}\right)^{-1}-\sum_{\mu<i}\gamma_\mu^2\left(\sum_k D_{i-k}\right)^{-1}\right\}\right.\\
&\qquad\left.-\gamma_{i+1}^2\left\{\sum_{\mu>i+1}\gamma_\mu^2\left(\sum_k D_{i+k}\right)^{-1}-\sum_{\mu<i+1}\gamma_\mu^2\left(\mathscr{D}+\sum_k \mathscr{D}_{i-k}\right)^{-1}\right\}\right](\delta B)^2.
\end{aligned} \tag{52}$$

Substituting (52) into (50) and neglecting terms of order higher than $(\delta B)^2$ eventually yields

$$\mathscr{P}(\mathscr{D}) = P(\mathscr{D})+\{G(\mathscr{D})P(\mathscr{D})+H(\mathscr{D})\,\mathrm{d}P(\mathscr{D})/\mathrm{d}\mathscr{D}+K\,\mathrm{d}^2P(\mathscr{D})/\mathrm{d}\,\mathscr{D}^2\}(\delta B)^2, \tag{53}$$

where

$$\begin{aligned}
G(\mathscr{D}) &= \left\langle\gamma_i^2\sum_{\mu>i}\gamma_\mu^2\left(\mathscr{D}+\sum_k D_{i+k}\right)^{-2}+\gamma_{i+1}^2\sum_{\mu<i+1}\gamma_\mu^2\left(\mathscr{D}+\sum_k D_{i-k}\right)^{-2}\right\rangle\\
&= 2\langle\gamma^2\rangle^2\int_0^\infty \exp(-\mathscr{D}s)\,s\{1-\bar{P}_D(s)\}^{-1}\,\mathrm{d}s,
\end{aligned} \tag{54}$$

$$\begin{aligned}
H(\mathscr{D}) &= \left\langle\gamma_i^2\left\{\sum_{\mu>i}\gamma_\mu^2\left(\mathscr{D}+\sum_k D_{i+k}\right)^{-1}\sum_{\mu<i}\gamma_\mu^2\left(\sum_k D_{i-k}\right)^{-1}\right\}\right.\\
&\qquad\left.-\gamma_{i+1}^2\left\{\sum_{\mu>i+1}\gamma_\mu^2\left(\sum_k D_{i+k}\right)^{-1}\sum_{\mu<i+1}\gamma_\mu^2\left(\mathscr{D}+\sum_k D_{i-k}\right)^{-1}\right\}\right\rangle\\
&= 2\langle\gamma^2\rangle^2\int_0^\infty \{\exp(-\mathscr{D}s)-1\}\{1-\bar{P}_D(s)\}^{-1}\,\mathrm{d}s,
\end{aligned} \tag{55}$$

and

$$K = \langle\gamma^4\rangle - \langle\gamma^2\rangle^2 . \tag{56}$$

It is quite clear from equation (53) that the distribution function has changed from the initial distribution function $P(D)$ to one which depends upon $\langle\gamma^2\rangle$ as well as $\langle D\rangle$. Therefore, if there exists some special value B_0 for which the level spacings and reduced widths are uncorrelated, then in general when $B \neq B_0$ correlations between spacings and widths must exist.

VI. Change in Parameters with Change in Radius

Let us consider the physical requirement that the collision function $\mathscr{S}$ given by equation (5) should be independent of the arbitrary radius a. Then from equations (5) and (6b) we obtain

$$\frac{\partial R}{\partial a} = \mathrm{i}\frac{\mathrm{d}\Omega}{\mathrm{d}a}\frac{1}{P\Omega}\{1-2(S-B)R+(S^2+P^2-2SB+B^2)R^2\}$$

$$-\frac{1}{P}\frac{\partial P}{\partial a}R\{1+(B-S)R\}-\frac{\partial S}{\partial a}R^2 . \tag{57}$$

We shall consider s-waves only where (Preston 1965)

$$P = ka = (2ME)^{\frac{1}{2}}a , \qquad S = 0 , \qquad \Omega^2 = \exp(-2\mathrm{i}ka) ,$$

from which we obtain

$$\frac{\partial R}{\partial a} = \frac{1}{a}+\left(\frac{B^2}{a}+2MaE-\frac{B}{a}\right)R^2-\frac{R}{a}(1-2B) . \tag{58}$$

However, using equation (1) we get

$$\frac{\partial R}{\partial a} = \sum_{\lambda}\frac{\partial\gamma_\lambda^2}{\partial a}\frac{1}{E_\lambda-E}-\sum_{\lambda}\frac{\gamma_\lambda^2}{(E_\lambda-E)^2}\frac{\partial E_\lambda}{\partial a}+\frac{\partial R_\infty}{\partial a} . \tag{59}$$

Substituting equation (1) into (58) and equating the residues of poles of each order in $E_\lambda-E$, we obtain the three equations for small R_∞

$$\partial E_\lambda/\partial a = -\gamma_\lambda^2\{2MaE_\lambda+B(B-1)/a\} , \tag{60a}$$

$$\partial\gamma_\lambda^2/\partial a = \gamma_\lambda^2\{(2B-1)/a-2Ma(\gamma_\lambda^2-2E_\lambda F_\lambda)\} , \tag{60b}$$

$$\partial R_\infty/\partial a = 1/a , \tag{60c}$$

where

$$F_\lambda = \sum_{\mu\neq\lambda}\gamma_\mu^2/(E_\lambda-E_\mu) , \qquad \langle F_\lambda\rangle = 0 . \tag{61}$$

The most common value for B chosen in s-states is $B = 0$, and for this value we obtain

$$\partial E_\lambda/\partial a = -2MaE_\lambda\gamma_\lambda^2 , \qquad \partial\gamma_\lambda^2/\partial a = 2Ma\gamma_\lambda^2(2E_\lambda F_\lambda-\gamma_\lambda^2)-\gamma_\lambda^2/a , \tag{62a, b}$$

with equation (60c) unchanged. Equation (62a) gives

$$\partial D_\lambda/\partial a = 2Ma\{E_\lambda\gamma_\lambda^2-E_{\lambda+1}\gamma_{\lambda+1}^2\} ,$$

that is,

$$\partial\langle D\rangle/\partial a = -2Ma\langle\gamma^2\rangle\langle D\rangle\,. \tag{63}$$

Next consider from equation (62b)

$$\langle\partial\gamma_\lambda^2/\partial a\rangle = \partial\langle\gamma^2\rangle/\partial a = \langle -2Ma\gamma_\lambda^4 + 4Ma\gamma_\lambda^2 E_\lambda F_\lambda - \gamma_\lambda^2/a\rangle\,. \tag{64}$$

The term containing E_λ can be shown to have a zero average and therefore we have by the methods of the previous section

$$\partial\langle\gamma^2\rangle/\partial a = -2Ma\langle\gamma^4\rangle - \langle\gamma^2\rangle/a\,. \tag{65}$$

For a Porter–Thomas distribution, equation (65) becomes

$$\partial\langle\gamma^2\rangle/\partial a = -6Ma\langle\gamma^2\rangle^2 - \langle\gamma^2\rangle/a\,. \tag{66}$$

Equation (66) has the unique solution

$$\langle\gamma^2(a)\rangle = a^{-1}(C+6Ma)^{-1}\,, \qquad C = \{a_0\langle\gamma^2(a_0)\rangle\}^{-1} - 6Ma_0\,, \tag{67}$$

where C is a constant of integration which is independent of a. Equations (67) give explicitly the dependence of the mean distribution of reduced widths on the matching radius a.

Returning to equation (63) and integrating with respect to a, we obtain the solution

$$\langle D(a)\rangle = \langle D(a_0)\rangle\{(C+6Ma_0)/(C+6Ma)\}^{\frac{1}{3}}\,. \tag{68}$$

The average level spacing $\langle D\rangle$ turns out to be a monotonic function of a, varying smoothly from the value at a_0 to zero as a becomes infinite. This can be seen from the following tabulation of the matching radius dependence on level spacing, where we have chosen $\langle D(a_0)\rangle = 1$, $a_0 = 1$, $C = 1$, $6M = 1$, and $\langle\gamma^2(a_0)\rangle = 0\cdot5$:

a	1·0	1·25	1·5	2·0	3·0	4·0	5·0	7·5	10	∞
$\langle D\rangle$	1·0	0·954	0·928	0·874	0·794	0·734	0·693	0·618	0·567	0
$\langle\gamma^2\rangle$	0·5	0·356	0·267	0·167	0·084	0·050	0·033	0·015	0·008	0

Finally, equation (60c) can be integrated to give approximately

$$R_\infty = \ln(a/a_0)\,, \tag{69}$$

where a_0 has been chosen as the nuclear radius, and therefore the constant background in equation (1) vanishes at this radius.

VII. Conclusions

Several methods have been used to illustrate that, contrary to current opinion, the statistical distributions of reaction matrix parameters do depend on both the choice of the boundary condition matrix **B** and the matching radius a. Explicit expressions for the changes in the moments of the distributions as well as for the changes in the distributions themselves have been derived. The two important examples of experimentally verified distributions considered have been shown to be non-invariant under the relevant transformations. We conclude therefore that the technique of statistically sampling reaction matrix parameters from such distributions in order to generate cross sections may be valid only for a particular value of **B** and a special matching radius.

In addition, if one were to analyse experimental data and derive sets of distributions of γ_λ^2 and E_λ, using ranges of values for a and B, one should find that these distributions depend upon a and B. By using a least-squares fit to a Porter–Thomas distribution and a Wigner distribution respectively, it should be possible to select an a and B which give the best fits. We speculate that the values obtained might be those where a is close to the nuclear radius and B is of order $-l$ (l being the orbital angular momentum), as this choice gives zero level shift at threshold for square-well potentials.

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