LA-4327

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Perturbation Transformation of Nuclear Cross-Section Parameters between Wigner-Eisenbud and Kapur-Peierls Formalisms: The PERTA Program

UNITED STATES
ATOMIC ENERGY COMMISSION
CONTRACT W-7405-ENG. 36

Printed in the United States of America. Available from
Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards, U. S. Department of Commerce
Springfield, Virginia 22151
Price: Printed Copy $3.00; Microfiche $0.65

Written: November 25, 1969

Distributed: January 7, 1970

LA-4327
UC-34, PHYSICS
TID-4500

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Donald R. Harris

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PERTURBATION TRANSFORMATION OF NUCLEAR CROSS-SECTION PARAMETERS BETWEEN WIGNER-EISENBUD AND KAPUR-PEIERLS FORMALISMS - THE PERTA PROGRAM

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ABSTRACT

The transformation between nuclear cross sections in the Wigner-Eisenbud and Kapur-Peierls formalisms is expressed by treating off-diagonal elements of the inverse level matrix as perturbations. A FORTRAN IV program, PERTA, is developed to compute the perturbation transformation. The applicability of the perturbation to real nuclei is tested for low-energy neutron cross sections of fissile nuclides. The perturbation transformation is applied to the study of properties of Kapur-Peierls parameters, namely, their probability distribution, the range in energy of interference effects, and the degree of asymmetry of resonant shapes of radiative capture cross sections.

I. INTRODUCTION

The Wigner-Eisenbud[1,2] and Kapur-Peierls[3,4] multilevel formalisms have been used extensively to interpret nuclear reaction phenomena and to fit observed cross sections. They have been used in preference to single-level resonance formulae to describe nucleon interactions with a wide range of nuclei, including oxygen, manganese, and fissile nuclides, for which multilevel interference effects are possibly or actually significant. Although these formalisms are consistent, and can be derived from each other,[1,5] their application is complementary. Expressions for cross sections in the Kapur-Peierls formalism are simply related with observed cross-section shapes. Moreover, in fitting Kapur-Peierls expressions to observed cross sections, knowledge is not required of numbers and characteristics of levels and channels. On the other hand, the parameters appearing in the Wigner-Eisenbud formalisms are directly related with nuclear wave functions. This fact permits inferences about the nuclear wave functions from observed Wigner-Eisenbud parameters, and it permits generalizations such as the Porter-Thomas plausibility argument[6] for the probability distribution of Wigner-Eisenbud parameters.

The exact transformation between sets of numbers parameterizing the two formalisms is well-defined,[1,5] and programs are available[4,7,8] for accurate numerical transformation from Wigner-Eisenbud to Kapur-Peierls parameter sets. The exact transformation, however, is not simple, and it is not easy to understand the action of the transformation, that is, of the interference mechanism. In particular, the joint probability distribution of Kapur-Peierls parameters has not been determined.

In the present study, an approximate but clearer transformation between the two formalisms is developed (Sec. II), tested (Sec. III and IV), and briefly applied (Sec. V) to clarification of certain properties of Kapur Peierls parameters, namely, their probability distribution, the range in energy of interference effects, and the degree of asymmetry of resonant shapes of radiative capture cross sections. This transformation, a perturbation transformation, is described in detail in the next section. The perturbation transformation proceeds from the Wigner-Eisenbud to the Kapur-Peierls parameter sets, but if the perturbation is indeed small the transformation can be inverted.

In the Wigner-Eisenbud formalism,[1,2] the total cross section, σ_{ct}, and the cross section for reaction from a channel c into a channel c', $\sigma_{cc'}$ are expressed as

$$\sigma_{ct} = \frac{2\pi}{k_c^2} \sum_{J\Pi} g_J \, \mathrm{Re}\left(1 - U_{cc}^{J\Pi}\right) \quad , \qquad (1)$$

and

$$\sigma_{cc'} = \frac{\pi}{k_c^2} \sum_{J\Pi} g_J \left| \delta_{cc'} - U_{cc'}^{J\Pi} \right| \quad . \qquad (2)$$

Here k_c is the wave number of the incident particle in channel c, and g_J is the statistical weight for states with angular momentum J and parity Π. The elements of the collision matirx $U^{J\Pi}$ are determined by the level matrix $A^{J\Pi}$

$$U_{cc'}^{J\Pi} = e^{i(\varphi_c + \varphi_{c'})} \left[\delta_{cc'} + i \sum_{\lambda,\lambda' \epsilon J\Pi} \Gamma_{\lambda c}^{1/2} A_{\lambda\lambda'}^{J\Pi} \Gamma_{\lambda' c}^{1/2} \right] \quad , \qquad (3)$$

where φ_c is the phase shift for potential scattering in channel c, and $\Gamma_{\lambda c}$ is the partial width for decay of level λ through channel c. By convention, $\Gamma_{\lambda c}^{1/2}$ is assigned the same algebraic sign as the corresponding reduced width amplitude.[9] Finally, the level matrix $A^{J\Pi}$ is defined in terms of its inverse

$$A_{\lambda\lambda'}^{J\Pi^{-1}} = (E_\lambda - E)\delta_{\lambda\lambda'} - \frac{i}{2} \sum_c \Gamma_{\lambda c}^{1/2} \Gamma_{\lambda' c}^{1/2} \quad , \qquad (4)$$

where E_λ, aside from a small level shift,[5] is the energy of a nuclear state.

The numerical and conceptual difficulties in practical application of the Wigner-Eisenbud formalism arise in part in the inversion of A^{-1} to obtain the level matrix A. A useful approximate inversion was developed by Thomas[10] using first order perturbation theory regarding the off-diagonal elements of A^{-1} as perturbations on the diagonal part. A similar technique is employed here, but perturbation theory is applied differently. The transformation between Wigner-Eisenbud and Kapur-Peierls parameter sets is facilitated by introduction of a complex orthogonal matrix S that diagonalizes the inverse level matrix A^{-1} to a diagonal matrix D. In Sec. II we develop the perturbation calculation of S and D, again regarding the off-diagonal elements of A^{-1} as perturbations on the diagonal part. This procedure is consistent with Thomas' analysis, and it can be shown that level matrices A computed by using the two approaches (we do not actually display a computed A in the perturbation transformation) differ only in terms of second and higher order in the perturbation.

The remaining problems in developing an intelligible transformation between Wigner-Eisenbud and Kapur-Peierls parameter sets are algebraic and numerical. In particular, it is not clear when terms of second and higher order in the (not always small) perturbation can be profitably discarded or retained. Some of these alternatives, and the general applicability of the perturbation transformation, are tested by use of the FORTRAN IV program PERTA, described in Sec. III. Results are presented in Sec. IV for a representative set of 31 levels in ^{235}U + n that exhibit both weak and moderatly strong level-level interference. We conclude that the perturbation results describe weakly interfering cross sections well and describe moderately strong interference qualitatively.

The perturbation analysis requires that the off-diagonal elements, $-i/2 \sum_c \Gamma_{\lambda c}^{1/2} \Gamma_{\lambda' c}^{1/2}$, of the inverse matrix be small in some sense compared with the diagonal elements, $E_\lambda - E - i/2\, \Gamma_\lambda$. A sufficient, but not necessary, condition for this requirement is that level widths are small compared with level spacings. Perhaps a more widely applicable condition for this requirement is a large degree of incoherence in the level parameters $\Gamma_{\lambda c}^{1/2}$. The extreme form of such incoherence is the assumption that for channels of a class c_I

$$\sum_{c\epsilon c_I} \Gamma_{\lambda c}^{1/2} \Gamma_{\lambda' c}^{1/2} = \Gamma_{\lambda c_I} \delta_{\lambda\lambda'} \quad . \qquad (5)$$

This condition is not precisely applicable to a nonvanishing, multichannel dyadic product, but it has been very useful in practical application of the Wigner-Eisenbud formalism.[9,11] Porter and others[6,10,12] have discussed the physical bases for incoherence. Here we regard the applicability of the present perturbation theory to be a question for experimental test.

It cannot be expected that the perturbation results will apply even qualitatively if multilevel interference is very strong, as has been suggested by Lynn[13] for certain fission processes. The present perturbation analysis provides a convenient test for strong interference in that to first order in the perturbation the level energy and total level width are unchanged in the transformation between Wigner-Eisenbud and Kapur-Peierls parameter sets. This is in marked contrast with the Lynn effect where interference is so strong that interfering Wigner-Eisenbud levels shift so much in the transformation to Kapur-Peierls parameters that they coalesce. An immediate test of possible applicability of the perturbation analysis to a particular set of cross sections is thus a test of approximate equality between level energies and total level widths in equivalent Wigner-Eisenbud and Kapur-Peierls parameter sets.

It will be shown that this test is satisfied for the $^{235}U + n$ cross sections studied here. De Saussure and Perez[7] have also reported Wigner-Eisenbud and Kapur-Peierls parameter sets, transformed by using the POLLA program,[7] for $^{233}U + n$, and again the test appears to be satisfied. If interference effects are moderate for such nuclei, then the perturbation transformation has greater applicability than might have been expected. Had very strong interference effects been observed then more accurate transformation equations might be developed by treating a few levels or channels exactly and applying a very approximate treatment to the remainder.[14-17,10] One of the conclusions of the present study (Sec. V) is that some interference effects are long range, varying as the inverse level spacing, and it can be conjectured that neighboring levels do not provide all significant interference effects. These results, the apparent absence of Lynn effects for certain important nuclei, and the long range of interference effects provide motivation for the study of multilevel interference effects by many-level, many-channel approximations.

II. THE PERTURBATION TRANSFORMATION

It is convenient to develop the perturbation transformation with reference to the diagonalizing procedure and notation of Adler and Adler,[18] although we do not yet wish to limit the incident particle to be an s-wave neutron. Let D represent a diagonal matrix. Then $A^{-1} + EI$, a complex symmetric matrix with components $E_\lambda \delta_{\lambda\lambda'} - \sum_c \Gamma_{\lambda c}^{1/2} \Gamma_{\lambda' c}^{1/2}$, is diagonalized to D by a complex orthogonal matrix S. That is,

$$(A^{-1} + EI)S = SD \quad . \tag{6}$$

Recalling that the inverse of an orthogonal matrix S is its transpose, S^{tr}, then

$$A^{-1} = S(D - EI)S^{tr} \quad , \tag{7}$$

and the inverse of A is readily obtained by

$$A = S(D - EI)^{-1} S^{tr} \quad . \tag{8}$$

To the extent that $A^{-1} + EI$ is insensitive to energy,[19] the diagonalizing matrix S will be also, and the energy dependence of the level matrix A is confined to the diagonal matrix $(D - EI)^{-1}$. Writing out Eq. (8),

$$A_{\lambda\lambda'} = \sum_k \frac{S_{\lambda k} S_{\lambda' k}}{D_{kk} - E} \quad , \tag{9}$$

and introducing this expression into Eq. (3), the collision matrix is obtained.

$$U_{cc'} = e^{i(\varphi_c + \varphi_{c'})} \left[\delta_{cc'} + i \sum_k \frac{\tilde{\Gamma}_{kc}^{1/2} \tilde{\Gamma}_{kc'}^{1/2}}{D_{kk} - E} \right] \quad , \tag{10}$$

where the complex width $\tilde{\Gamma}_{kc}$ for level k and channel c is defined by

$$\tilde{\Gamma}_{kc}^{1/2} = \sum_\lambda S_{\lambda k} \Gamma_{\lambda c}^{1/2} \quad . \tag{11}$$

Cross sections can then be obtained from Eqs. (1) and (2) by application of the lemma of App. A. First, however, the present perturbation technique is described in some detail.

Let B represent the matrix $A^{-1} + EI$, and suppose B can be decomposed into parts $\hat{B} + \delta B$, where δB is a small perturbation. Let $\hat{S}$ represent the matrix that diagonalizes $\hat{B}$ to $\hat{D}$, and let $\hat{S} + \delta S$ represent the matrix that diagonalizes $\hat{B} + \delta B$ to $\hat{D} + \delta D$. In App. B, a perturbation theory for symmetric matrices is developed, and expressions are obtained for δD [Eq. (B-7)] and for δS [Eq. (B-15)] to first order in the perturbation.

$$\delta D_{kk} = \sum_{\lambda,\lambda'} \hat{S}_{\lambda k}\, \delta B_{\lambda\lambda'}\, \hat{S}_{\lambda' k} \quad , \tag{12}$$

and

$$\delta S_{jk} = \sum_{\lambda \neq k} \frac{\sum_{\lambda',\lambda''} \hat{S}_{\lambda'\lambda}\, \delta B_{\lambda'\lambda''}\, \hat{S}_{\lambda'' k}}{\hat{D}_{kk} - \hat{D}_{\lambda\lambda}}\, \hat{S}_{j\lambda} \quad . \tag{13}$$

In a previous study, the perturbation was taken to be the energy-dependent particle channel contributions to the inverse level matrix.[19] Here we take the unperturbed $\hat{B}$ to be the diagonal part of $A^{-1} + EI$, while δB is the off-diagonal part.

$$\hat{B}_{\lambda\lambda'} = (E_\lambda - E - \tfrac{i}{2}\Gamma_\lambda)\delta_{\lambda\lambda'} \quad , \tag{14}$$

and

$$\delta B_{\lambda\lambda'} = -\frac{i}{2} \sum_c \Gamma_{\lambda c}^{1/2}\, \Gamma_{\lambda' c}^{1/2}\, (1 - \delta_{\lambda\lambda'}) \quad . \tag{15}$$

In this case a great simplification emerges in that $\hat{B}$ is already diagonal, so that $\hat{S}$ is the identity matrix I, and $\hat{D}$ equals $\hat{B}$. Thus, from Eqs. (12) through (15),

$$\delta D_{kk} = 0 \quad , \tag{16}$$

and

$$\delta S_{jk} = \frac{-\frac{i}{2} \sum_c \Gamma_{jc}^{1/2}\Gamma_{kc}^{1/2}(1 - \delta_{jk})}{(E_k - E_j) - \frac{i}{2}(\Gamma_k - \Gamma_j)} \quad . \tag{17}$$

The complex level widths $\tilde{\Gamma}_{kc}$ are obtained from Eqs. (11) and (17),

$$\tilde{\Gamma}_{kc}^{1/2} = \Gamma_{kc}^{1/2} \left[1 + \sum_{\substack{\lambda \in J\Pi \\ \lambda \neq k}} \frac{\Gamma_{\lambda c}^{1/2}}{\Gamma_{kc}^{1/2}} \left(F_{\lambda k}^1 + i\, F_{\lambda k}^2 \right) \right] \quad , \tag{18}$$

where

$$F_{\lambda k}^1 = \frac{(\Gamma_k - \Gamma_\lambda)/2}{(E_k - E_\lambda)^2 + (\Gamma_k - \Gamma_\lambda)^2/4}\, \frac{1}{2} \sum_{c'} \Gamma_{\lambda c'}^{1/2}\, \Gamma_{kc'}^{1/2} \, , \tag{19}$$

and

$$F_{\lambda k}^2 = \frac{(E_\lambda - E_k)}{(E_k - E_\lambda)^2 + (\Gamma_k - \Gamma_\lambda)^2/4}\, \frac{1}{2} \sum_{c'} \Gamma_{\lambda c'}^{1/2}\, \Gamma_{kc'}^{1/2} \, . \tag{20}$$

The operations expressed thus far in this section refer to levels of a particular spin-parity sequence. To illustrate, the k^{th} level referred to in Eq. (18) is a member of a particular spin-parity sequence $J\Pi$ ($k \epsilon J\Pi$). Levels of the $J\Pi$ sequence interfere with one another and only these contribute to the perturbation of $\tilde{\Gamma}_{kc}$.

Cross sections can be expressed conveniently in terms of parameters $M_{cc'}^{kj}$, which we refer to as fractional perturbations. For the level $k(k\epsilon J\Pi)$, for channels c and c′, and for j = 1, 2,

$$M_{cc'}^{kj} \equiv \sum_{\substack{\lambda \epsilon J\Pi \\ \lambda \neq k}} \left(\frac{\Gamma_{\lambda c}^{1/2}}{\Gamma_{kc}^{1/2}} + \frac{\Gamma_{\lambda c'}^{1/2}}{\Gamma_{kc'}^{1/2}} \right) F_{\lambda k}^j \quad . \tag{21}$$

The fractional perturbation $M_{cc'}^{kj}$ is symmetric in c and c′, and has the property that

$$M_{cc'}^{kj} = \frac{1}{2}\left(M_{cc}^{kj} + M_{c'c'}^{kj} \right) \quad . \tag{22}$$

Further discussion of these parameters will be deferred until cross sections are expressed in terms of them.

The perturbed level widths are, in terms of fractional perturbations,

$$\tilde{\Gamma}_{kc}^{1/2} = \Gamma_{kc} \left[1 + \frac{1}{2}\left(M_{cc}^{k1} + i\, M_{cc}^{k2} \right) \right] \quad . \tag{18'}$$

The perturbed collision matrix $U_{cc'}^{J\Pi}$ is obtained by substituting Eq. (18′) into Eq. (10) and applying Eq. (22), so that

$$U_{cc'}^{J\Pi} = e^{i(\varphi_c + \varphi_{c'})} \left\{ \delta_{cc'} + i \sum_{k \epsilon J\Pi} \frac{\Gamma_{kc}^{1/2}\, \Gamma_{kc'}^{1/2} \left[1 + R_{cc'}^{k1} + i R_{cc'}^{k2} \right]}{E_k - E - i\,\Gamma_k/2} \right\} , \tag{23}$$

where

$$R_{cc'}^{k1} = M_{cc'}^{k1} + \frac{1}{4}\left(M_{cc}^{k1}\, M_{c'c'}^{k1} - M_{cc}^{k2}\, M_{c'c'}^{k2} \right) \quad , \tag{24}$$

and

$$R_{cc'}^{k2} = M_{cc'}^{k2} + \frac{1}{4}\left(M_{cc}^{k1}\, M_{c'c'}^{k2} + M_{cc}^{k2}\, M_{c'c'}^{k1} \right) \quad . \tag{25}$$

Later, we numerically test the adequacy of approximating $R_{cc'}^{kj}$ by the linear term $M_{cc'}^{kj}$ by using the PERTA program. In Eq. (10), D_{kk} has been replaced by its unperturbed value $\mathfrak{D}_{kk}$ or $E_k - i\Gamma_k/2$. The remarkable fact that to first order in the perturbation the level energy E_k and total level width Γ_k are unchanged according to Eq. (16) permits identification of Wigner-Eisenbud levels and Kapur-Peierls levels. In the presence of strong interference, such identification is not simple.[13] The invariance of E_k and $\Gamma_k/2$ in the perturbation transformation is, of course, a much stronger statement than the well known invariance of $\sum_k E_k$ and $\sum_k \Gamma_k/2$ resulting from the invariance of the trace of the matrix $A^{-1} + EI$ in the orthogonal transformation [Eq. (6)].

A. Total Cross Section

The total cross section σ_{ct} results from substitution of the expression of Eq. (23), for the perturbed collision matrix into Eq. (1), noting that $\sum_J g_J$ is unity.

$$\sigma_{ct} = \frac{4\pi}{k_c^2} \sin^2 \varpi_c$$

$$+ \frac{2\pi}{k_c^2} \sum_{J\Pi} g_J \sum_{k\epsilon J\Pi} \frac{\Gamma_{kc}\left\{\frac{\Gamma_k}{2}\left[\left(1 + R_{cc}^{k1}\right) \cos 2\varpi_c - R_{cc}^{k2} \sin 2\varpi_c\right] + (E_k - E)\left[\left(1 + R_{cc}^{k1}\right) \sin 2\varphi_c + R_{cc}^{k2} \cos 2\varpi_c\right]\right\}}{(E_k - E)^2 + \Gamma_k^2/4} . \tag{26}$$

For s-wave neutrons, a widely used notation introduced by the Adlers[18,7] is

$$\sigma_{nt} = \frac{4\pi}{k_n^2} \sin^2 k_n a_n + \frac{1}{E^{1/2}} \sum_{J\Pi} \sum_{k\epsilon J\Pi} \frac{\nu_k G_k^T + (\mu_k - E) H_k^T}{(\mu_k - E)^2 + \nu_k^2} , \tag{27}$$

$$G_k^T \equiv \alpha_k \cos 2k_n a_n + \beta_k \sin 2k_n a_n , \tag{28}$$

and

$$H_k^T \equiv \beta_k \cos 2k_n a_n - \alpha_k \sin 2k_n a_n . \tag{29}$$

A necessary modification to their notation has been introduced in that we explicitly sum over each level in a particular spin-parity sequence, then over all sequences. The neutron phase shift ϖ_n is taken to be $-k_n$ times the neutron channel radius a_n, and the neutron width Γ_{kn} is expressed as $\Gamma_{kn}^o E^{1/2}$. Comparing Eqs. (27), (28), and (29) with Eq. (26), we obtain the first-order perturbation transformation from Wigner-Eisenbud to Kapur-Peierls total cross section parameters for the level $k(k\epsilon J\Pi)$,

$$\alpha_k = \frac{2\pi E}{k_n^2} g_J \Gamma_{kn}^o \left(1 + R_{nn}^{k1}\right) , \tag{30}$$

$$\beta_k = \frac{2\pi E}{k_n^2} g_J \Gamma_{kn}^o R_{nn}^{k2} , \tag{31}$$

$$\mu_k = E_k , \tag{32}$$

and

$$\nu_k = \frac{\Gamma_k}{2} . \tag{33}$$

The parameters R_{cc}^{kj} contain the effect of the perturbation on total cross section, which otherwise has the usual Breit-Wigner form. It can be seen from Eqs. (24) and (25) that the parameters R_{cc}^{kj} depend on the fractional perturbations M_{cc}^{kj}, and, indeed, approximate them when they are small compared to unity.

Reference to the definition of fractional perturbations, Eq. (21), shows that they tend to be larger for weak levels, specifically, M_{cc}^{kj} varies as $1/\Gamma_{kc}^{1/2}$. Moreover, the presence of other strong levels increases $|M_{cc}^{kj}|$, although their effect has a rather weak dependence on level energy separation, varying as $(E_k - E_\lambda)^{-1}$ for M_{cc}^{k2} and as $(E_k - E_\lambda)^{-2}$ for M_{cc}^{k1}. Finally, a nearby strong level will have little effect on M_{cc}^{k1} if Γ_k approximately equals Γ_λ, and it will have little perturbation effect at all if $\sum_c \Gamma_{\lambda c}^{1/2} \Gamma_{kc}^{1/2}$ is small.

B. Reaction Cross Sections

The reaction cross-section $\sigma_{cc'}$, $c \neq c'$, is obtained by substituting Eq. (23) into Eq. (2), applying Eq. (22), and ignoring terms of second order in the perturbation,

$$\sigma_{cc'} = \frac{\pi}{k_c^2} \sum_{J\Pi} g_J \sum_{k,k'\epsilon J\Pi} \frac{\Gamma_{kc}^{1/2}\Gamma_{kc'}^{1/2}\Gamma_{k'c}^{1/2}\Gamma_{k'c'}^{1/2} \left[1 + Q_{cc}^{kk'1} + i\, Q_{cc}^{kk'2}\right]}{(E_k - E - i\Gamma_k/2)(E_{k'} - E + i\Gamma_{k'}/2)} \quad . \tag{34}$$

This expression can be simplified by use of the lemma of App. A.

$$\sigma_{cc'} = \frac{\pi}{k_c^2} \sum_{J\Pi} g_J \sum_{k\epsilon J\Pi} \frac{A_{cc'}^k - B_{cc'}^k (E_k - E)}{(E_k - E)^2 + \Gamma_k^2/4} \quad , \tag{35}$$

where $A_{cc'}^k$, or $A_k + E_k B_k$ of App. A is

$$A_{cc'}^k = \Gamma_{kc}\Gamma_{kc'}\left(1 + Q_{cc'}^{kk1}\right) + \Gamma_k \sum_{\substack{k'\epsilon J\Pi \\ k'\neq k}} \frac{\Gamma_{kc}^{1/2}\Gamma_{kc'}^{1/2}\Gamma_{k'c}^{1/2}\Gamma_{k'c'}^{1/2} \left[\left(1 + Q_{cc'}^{kk'1}\right)(\Gamma_k + \Gamma_{k'})/2 - Q_{cc'}^{kk'2} (E_k - E_{k'})\right]}{(E_k - E_{k'})^2 + (\Gamma_k + \Gamma_{k'})^2/4} \quad , \tag{36}$$

and

$$B_{cc'}^k = 2 \sum_{k'\epsilon J\Pi} \frac{\Gamma_{kc}^{1/2}\Gamma_{kc'}^{1/2}\Gamma_{k'c}^{1/2}\Gamma_{k'c'}^{1/2} \left[\left(1 + Q_{cc'}^{kk'1}\right)(E_k - E_{k'}) + Q_{cc'}^{kk'2} (\Gamma_k + \Gamma_{k'})/2\right]}{(E_k - E_{k'})^2 + (\Gamma_k + \Gamma_{k'})^2/4} \quad . \tag{37}$$

Here

$$Q_{cc}^{kk'1} = R_{cc'}^{k1} + R_{cc'}^{k2} + R_{cc'}^{k1} R_{cc'}^{k'1} + R_{cc'}^{k2} R_{cc'}^{k'2} \quad , \tag{38}$$

$$Q_{cc'}^{kk'2} = R_{cc'}^{k2} - R_{cc'}^{k'2} + R_{cc'}^{k2} R_{cc'}^{k'1} - R_{cc'}^{k1} R_{cc'}^{k'2} \quad , \tag{39}$$

and if the fractional perturbations are small compared with unity, then approximately

$$Q_{cc'}^{kk'1} = M_{cc'}^{k1} + M_{cc'}^{k'1} \quad , \tag{40}$$

and

$$Q_{cc'}^{kk'2} = M_{cc'}^{k2} - M_{cc'}^{k'2} \quad . \tag{41}$$

Again, we numerically test this approximation later by use of the PERTA program. Again, the parameters $M_{cc'}^{kj}$ act as fractional perturbations, and their magnitudes are governed by the same considerations as noted before. Let us list these considerations as they apply to the fractional perturbations $M_{cc'}^{kj}$:

a. Both $M_{cc'}^{k1}$ and $M_{cc'}^{k2}$ tend to be large (of either sign) when the level k is weak in the incoming (Γ_{kc} small) or outgoing ($\Gamma_{kc'}$ small) channel, or both.

b. Both $M_{cc'}^{k1}$ and $M_{cc'}^{k2}$ tend to be large (of either sign) when one or more other levels in the same $J\Pi$ sequence are strong in either the incoming or outgoing channels, or both.

c. The dependence of $M_{cc'}^{kj}$ contributions on level separation is rather weak, varying approximately as $(E_k - E_\lambda)^{-1}$ for $M_{cc'}^{k2}$, and as $(E_k - E_\lambda)^{-2}$ for $M_{cc'}^{k1}$.

d. Even a strong level may only weakly perturb a nearby weak level if $\sum_c \Gamma_{kc}^{1/2}\, \Gamma_{\lambda c}^{1/2}$ is small for this pair of levels, or (through $M_{cc'}^{k1}$) if the levels have nearly equal total widths.

e. When, as is often the case, level widths are smaller than level spacings (ΔE), $F_{\lambda k}^2$ and hence $M_{cc'}^{k2}$ tend to be larger than $F_{\lambda k}^1$ and $M_{cc'}^{k1}$ by an order of magnitude in $\Gamma/\Delta E$.

Although the fractional perturbations, $M_{cc'}^{kj}$, are descriptive and compact, they suffer in their definition from a difficulty that appears clerical but is in fact more interesting. If $\Gamma_{kc}^{1/2}$ or $\Gamma_{kc'}^{1/2}$ is small or zero, then $M_{cc'}^{kj}$ is very large or singular. The actual magnitude of the perturbation

$$P_{cc'}^{kk'j} \equiv \Gamma_{kc}^{1/2}\Gamma_{kc'}^{1/2}\Gamma_{k'c}^{1/2}\Gamma_{k'c'}^{1/2} M_{cc'}^{kj} \tag{42}$$

remains finite or vanishes, so that the effect on cross sections is finite or zero. A large fractional perturbation implies only that there can be a violent fractional effect of interference on a weak channel. The clerical difficulty created by a zero value of $\Gamma_{kc}^{1/2}$ can be circumvented by adding a negligible but finite increment to $\Gamma_{kc}^{1/2}$, and this device is employed in the PERTA program described later. Such a zero value of Γ_{kc} might be adopted for convenience in a cross-section fit. On the other hand, physical considerations suggest that a channel c might be closed at one level k ($\Gamma_{kc} = 0$) and yet be open at some other levels of the same $J\Pi$ sequence if the state k has some further, not yet defined, quantum number that is not suitable for the reaction to proceed through channel c.

C. Fission and Radiative Capture of s-Wave Neutrons

Cross sections for fission and radiative capture of s-wave neutrons can be expressed in the Adlers' notation,[18,7]

$$\sigma_{nf} = \frac{1}{E^{1/2}} \sum_{J\Pi} \sum_{k\epsilon J\Pi} \frac{\nu_k G_k^f + (\mu_k - E) H_k^f}{(\mu_k - E)^2 + \nu_k^2} \quad , \tag{43}$$

and

$$\sigma_{n\gamma} = \frac{1}{E^{1/2}} \sum_{J\Pi} \sum_{k\epsilon J\Pi} \frac{\nu_k G_k^\gamma + (\mu_k - E) H_k^\gamma}{(\mu_k - E)^2 + \nu_k^2} \quad . \tag{44}$$

The parameters μ_k and ν_k are equal to level energy and $\Gamma_k/2$ as is described by Eqs. (30) and (31). In the case of fission, the parameters F_k^f and H_k^f are expressed as sums of contributions from various fission channels , $c\epsilon f$,

$$G_k^f = \sum_{c\epsilon f} G_k^c \quad , \tag{45}$$

and

$$H_k^f = \sum_{c\epsilon f} H_k^c \quad , \tag{46}$$

where, comparing Eq. (43) with Eqs. (35) through (37),

$$G_k^c = \frac{2\pi E}{k_n^2} g_J \left\{ \frac{\Gamma_{kn}^o \Gamma_{kc}}{\Gamma_k} \left(1 + 2 M_{nc}^{k1}\right) + \sum_{\substack{k'\epsilon J\Pi \\ k' \neq k}} \frac{\Gamma_{kn}^{o1/2} \Gamma_{kc}^{1/2} \Gamma_{k'n}^{o1/2} \Gamma_{k'c}^{1/2} \left[\left(1 + M_{nc}^{k1} + M_{nc}^{k'1}\right) (\Gamma_k + \Gamma_{k'})/2 - \left(M_{nc}^{k2} - M_{nc}^{k'2}\right)(E_k - E_{k'})\right]}{(E_k - E_{k'})^2 + (\Gamma_k + \Gamma_{k'})^2/4} \right\} \tag{47}$$

$$-H_k^c = \frac{2\pi E}{k_n^2} g_J \sum_{\substack{k'\epsilon J\Pi \\ k' \neq k}} \frac{\Gamma_{kn}^{o1/2} \Gamma_{kc}^{1/2} \Gamma_{k'n}^{o1/2} \Gamma_{k'c}^{1/2} \left[\left(1 + M_{nc}^{k1} + M_{nc}^{k'1}\right)(E_k - E_{k'}) + \left(M_{nc}^{k2} - M_{nc}^{k'2}\right)(\Gamma_k + \Gamma_{k'})/2\right]}{(E_k - E_{k'})^2 + (\Gamma_k + \Gamma_{k'})^2/4} \quad . \tag{48}$$

These expressions describe the cross sections for neutron reaction into any channel c, whether this be a fission channel, a particle emission channel, or a radiation channel.

In particular, the cross section for radiative capture through one or a few channels is expressed as for fission.

$$G_k^\gamma = \sum_{c\epsilon\gamma} G_k^c \quad , \tag{49}$$

and

$$H_k^\gamma = \sum_{c\epsilon\gamma} H_k^c \quad . \tag{50}$$

However, the total radiative capture cross section through many channels is usefully expressed in a different way by use of the incoherence approximation of Eq. (5) for radiative channels, where

$$\sum_{c\epsilon\gamma} \Gamma_{kc}^{1/2} \Gamma_{k'c}^{1/2} = \Gamma_{k\gamma} \delta_{kk'} \quad . \tag{51}$$

When this approximation is made

$$\sum_{c\epsilon\gamma} \Gamma_{kn}^{o1/2} \Gamma_{kc}^{1/2} \Gamma_{k'n}^{o1/2} \Gamma_{k'c}^{1/2} M_{nc}^{kj} = \Gamma_{kn}^o \Gamma_{k\gamma} \frac{1}{2} M_{nn}^{kj} \delta_{kk'} - \Gamma_{kn}^{o1/2} \Gamma_{k'n}^{o1/2} \Gamma_{k'\gamma} F_{kk'}^j (1 - \delta_{kk'}), \tag{52}$$

and by using this relation, G_k^γ and H_k^γ can be expressed as

$$G_k^{\gamma} = \frac{2\pi E}{k_n^2} g_J \left\{ \frac{\Gamma_{kn}^{o}\Gamma_{k\gamma}}{\Gamma_k} \left(1 + M_{nn}^{kl}\right) \right.$$

$$\left. + \sum_{\substack{k' \epsilon J\Pi \\ k' \neq k}} \frac{\Gamma_{kn}^{o1/2}\Gamma_{k'n}^{o1/2}\left[F_{kk'}^{1}(\Gamma_{k\gamma} - \Gamma_{k'\gamma})(\Gamma_k + \Gamma_{k'})/2 + F_{kk'}^{2}(\Gamma_{k\gamma} + \Gamma_{k'\gamma})(E_k - E_{k'})\right]}{(E_k - E_{k'})^2 + (\Gamma_k + \Gamma_{k'})^2/4} \right\} \tag{53}$$

$$- H_k^{\gamma} = \frac{2\pi E}{k_n^2} g_J \sum_{\substack{k' \epsilon J\Pi \\ k' \neq k}} \frac{\Gamma_{kn}^{o1/2}\Gamma_{k'n}^{o1/2}\left[F_{kk'}^{1}(\Gamma_{k\gamma} - \Gamma_{k'\gamma})(E_k - E_{k'}) - F_{kk'}^{2}(\Gamma_{k\gamma} + \Gamma_{k'\gamma})(\Gamma_k + \Gamma_{k'})/2\right]}{(E_k - E_{k'})^2 + (\Gamma_k + \Gamma_{k'})^2/4} \quad . \tag{54}$$

These results for radiative capture of s-wave neutrons complete our development of expressions for cross sections by first-order perturbation of the inverse level matrix. Similar, more accurate expressions might be obtained by second-order perturbation of the inverse level matrix.

III. THE PERTA PROGRAM

The PERTA program, in FORTRAN IV for the CDC-6600, computes the perturbation transformation from input Wigner-Eisenbud parameters to Kapur-Peierls parameters in the Adler form. The program was devised to test aspects of the perturbation transformation and has extensive edits. Input and output are described in App. C. The program computes and edits the imaginary part of the inverse level matrix, Eq. (4); M_{nn}^{kl} and M_{nn}^{k2}, Eq. (21); R_{nn}^{kl} and R_{nn}^{k2}, Eqs. (24) and (25); M_{nc}^{kl} and M_{nc}^{k2} for fission channels c, Eq. (21); R_{nc}^{kl} and R_{nc}^{k2} for fission channels c, Eqs. (24) and (25); and the quantities appearing in Eqs. (27) through (29), Eqs. (45) through (48), and Eqs. (53) and (54). The program also computes and edits an area factor and tilt factor for each cross section, for example, for the total cross section

$$ART_k = G_k^T / G_k^T \text{ (single level formula)} \quad , \tag{55}$$

and

$$TT_k = H_k^T / G_k^T \quad . \tag{56}$$

Similar area and tilt factors are computed and edited for each fission channel, for all fission, and for radiative capture.

Input parameters control the approximations used for R_{nn}^{kj} in Eqs. (24) and (25) and for $Q_{nc}^{kk'j}$ (cc fission) in Eqs. (38) through (41).

IV. NUMERICAL RESULTS

The numerical results chosen for presentation here are based on the Wigner-Eisenbud parameters for 31 levels determined by Cramer[20] in a Reich-Moore[11] fit to measured ^{235}U (n,fission) cross sections. Inspection of these parameters, which are listed in Table I, suggests that level-level interference is expected not to be strong except in the neighborhoods of 26 and 45 eV. Table II demonstrates the perturbation transformation prediction that level energies and total level widths are approximately unchanged. The Adler parameters listed in Table II were computed by the POLLA program of de Saussure and Perez.[7] It is not known why $\sum_k E_k$ fails to equal $\sum_k \mu_k$ as is required by the invariance of the trace of a matrix under the transformation [Eq. (6)], which we noted earlier.

In Table III are listed the total cross-section parameters α_k and β_k as computed by POLLA.[7] These are compared with various PERTA approximations. The right-hand column shows that with zero perturbation ($M_{nn}^{kj} = 0$), the value of β_k is erroneously computed to be zero. From the central columns of Table III it appears that retaining terms quadratic in M_{nn}^{kj} in the express for R_{nn}^{kj} [Eqs. (24) and (25)] does not obviously improve the accuracy of the calculation. This is not unexpected, because in the perturbation inversion of A^{-1} terms of second and higher orders in the perturbation have been discarded. Consequently, introducing such terms into the later calculation of R_{nn}^{kj} need not improve the result.

Inspection of Table IV shows that for this set of levels in ^{235}U + n the inclusion of terms other

TABLE I

RESONANCE PARAMETERS FOR 3^- LEVELS IN $^{235}U + n$ (CRAMER[20] DATA)*

Level Energy (eV)	Reduced Neutron Width ($eV^{1/2} \times 10^3$)	Partial Widths for Fission in Two Channels (eV)	
E_k	Γ^o_{kn}	Γ_{kf1}	Γ_{kf2}
16.67	0.06	-0.085	0
18.05	0.098	+0.140	0
19.295	0.56	0	-0.065
20.19	0.0085	+0.050	0
20.67	0.04	0	+0.030
21.085	0.29	+0.023	0
22.950	0.095	-0.038	0
23.440	0.15	+0.014	0
23.620	0.122	0	-0.090
24.245	0.05	0	-0.055
25.62	0.22	0	+0.610
26.15	0.0015	0	-0.60
26.51	0.105	0	+0.225
27.18	0.011	+0.075	0
27.8	0.115	+0.075	0
28.42	0.028	-0.100	0
28.73	0.0062	+0.070	0
30.88	0.08	0	+0.020
31.55	0.003	0	-0.040
32.07	0.3	0	+0.042
33.52	0.29	0	+0.022
44.64	0.125	+0.175	0
45.04	0.055	0	-0.300
45.78	0.027	0	+0.100
46.65	0.046	+0.035	0
51.60	0.067	+0.060	0
52.22	0.33	0	-0.300
58.68	0.169	0	+0.115
60.22	0.134	0	-0.200
63.80	0.07	0	+0.250
68.40	0.017	0	-0.070

$^*g = 0.5$, $\Gamma_\gamma = 0.029$ eV

TABLE II

COMPARISON OF LEVEL ENERGIES AND WIDTHS IN WIGNER-EISENBUD AND KAPUR-PEIERLS FORMALISMS FOR 31 LEVELS IN $^{235}U + n$ (CRAMER DATA)

Wigner-Eisenbud[20]					
Level Energy (eV)	Level Width (eV)	Adler[7] Parameters (eV)		Differences (eV)	
E_k	Γ_k	μ_k	$2\nu_k$	$E_k - \mu_k$	$\Gamma_k - 2\nu_k$
16.67	0.1142	16.67	0.114	0.00	0.000
18.05	0.1694	18.05	0.170	0.00	-0.001
19.295	0.0965	19.30	0.096	0.00	0.001
20.19	0.0790	20.19	0.080	0.00	-0.001
20.67	0.0592	20.67	0.058	0.00	0.001
21.085	0.0533	21.08	0.054	0.00	-0.001
22.95	0.0675	22.95	0.068	0.00	0.000
23.44	0.0437	23.44	0.044	0.00	0.000
23.62	0.1196	23.63	0.114	-0.01	0.006
24.245	0.0842	24.25	0.082	0.00	0.002
25.62	0.6401	25.67	0.678	-0.05	-0.038
26.15	0.0890	26.14	0.088	0.01	0.001
26.51	0.2545	26.46	0.226	0.05	0.029
27.18	0.1041	27.18	0.104	0.00	0.000
27.80	0.1046	27.80	0.106	0.00	-0.001
28.42	0.1292	28.42	0.132	0.00	-0.003
28.73	0.0990	28.72	0.096	0.01	0.003
30.88	0.0494	30.88	0.050	0.00	-0.001
31.55	0.0690	31.55	0.070	0.00	-0.001
32.07	0.0727	32.07	0.072	0.00	0.001
33.52	0.0527	33.52	0.052	0.00	0.001
44.64	0.2048	44.64	0.204	0.00	0.001
45.04	0.3294	45.05	0.332	-0.01	-0.003
45.78	0.1292	45.77	0.126	0.00	0.003
46.65	0.0643	46.65	0.064	0.00	0.000
51.60	0.0895	51.60	0.090	0.00	0.000
52.22	0.3314	52.22	0.332	0.00	-0.001
58.68	0.1453	58.68	0.146	0.00	-0.001
60.22	0.2300	60.21	0.230	0.01	0.000
63.80	0.2796	63.79	0.278	0.01	0.002
68.40	0.0991	68.40	0.098	0.00	0.001
			Sums	0.03	0.000

TABLE III

COMPARISON OF α_k AND β_k COMPUTED IN VARIOUS APPROXIMATIONS FOR 31 LEVELS IN $^{235}U + n$ (CRAMER DATA)

Level Energy (eV)	POLLA Calculation		PERTA (All powers of M_{nn}^{kj} retained in R_{nn}^{kj})		PERTA (R_{nn}^{kj} Linear in M_{nn}^{kj})		PERTA (M_{nn}^{kj} set Equal to Zero)	
E_k	α_k	β_k	α_k	β_k	α_k	β_k	α_k	β_k
16.67	39.34	- 5.66	38.97	- 5.94	39.19	- 5.93	39.12	0.0
18.05	63.56	8.10	63.61	8.35	63.88	8.35	63.90	0.0
19.295	366.35	- 8.52	365.36	- 9.01	365.42	- 9.01	365.12	0.0
20.190	5.87	0.99	5.50	1.02	5.55	1.02	5.54	0.0
20.67	25.39	4.38	25.83	4.48	26.02	4.48	26.08	0.0
21.085	189.17	- 1.92	189.02	- 1.65	189.03	- 1.65	189.08	0.0
22.95	61.85	- 2.22	61.83	- 2.42	61.85	- 2.42	61.94	0.0
23.44	97.85	3.35	97.77	3.48	97.80	3.48	97.80	0.0
23.62	83.15	-12.88	80.92	-13.63	81.48	-13.46	79.54	0.0
24.245	34.90	-18.81	31.79	-18.66	34.30	-18.19	32.60	0.0
25.62	146.70	70.78	139.49	67.40	147.18	66.53	143.44	0.0
26.15	0.26	0.93	4.66	0.35	3.29	0.16	0.98	0.0
26.51	59.59	-30.63	57.01	-24.87	59.30	-26.65	68.46	0.0
27.18	6.98	2.13	7.01	2.19	7.18	2.19	7.17	0.0
27.80	75.81	- 7.08	74.93	- 6.78	75.08	- 6.76	74.98	0.0
28.42	17.63	3.79	17.86	3.56	18.03	3.58	18.26	0.0
28.73	3.93	0.70	4.12	0.73	4.15	0.72	4.04	0.0
30.88	52.24	0.64	52.03	0.51	52.03	0.51	52.16	0.0
31.55	1.77	- 0.83	3.85	- 1.22	3.94	- 1.22	3.91	0.0
32.07	195.88	- 2.17	195.46	- 1.42	195.46	- 1.42	195.60	0.0
33.52	188.60	- 8.07	188.89	- 7.91	188.97	- 7.91	189.08	0.0
44.64	81.62	1.83	81.56	2.10	81.57	2.10	81.50	0.0
45.04	35.22	- 0.15	35.09	- 0.16	35.09	- 0.16	35.86	0.0
45.78	17.96	3.45	18.25	3.40	18.40	3.32	17.60	0.0
46.65	29.90	- 1.87	29.89	- 1.85	29.92	- 1.85	29.99	0.0
51.60	43.61	- 1.41	43.64	- 1.30	43.65	- 1.30	43.68	0.0
52.22	215.44	- 0.24	215.13	- 0.73	215.13	- 0.73	215.16	0.0
58.68	110.25	- 4.20	110.44	- 4.13	110.48	- 4.12	110.19	0.0
60.22	87.14	2.91	87.09	2.72	87.11	2.72	87.37	0.0
63.80	45.75	2.44	45.60	2.47	45.64	2.47	45.64	0.0
68.40	11.10	0.26	11.09	0.24	11.09	0.24	11.08	0.0

TABLE IV

COMPARISON OF KAPUR-PEIERLS FISSION PARAMETERS IN VARIOUS APPROXIMATIONS FOR 31 LEVELS IN ^{235}U (CRAMER DATA)

Level Energy (eV)	POLLA Calculation		PERTA (All Powers of M)		PERTA (Linear in M)	
E_k	$G_k^F(BeV^{3/2})$	$H_k^F(BeV^{3/2})$	$G_k^F(BeV^{3/2})$	$H_k^F(BeV^{3/2})$	$G_k^F(BeV^{3/2})$	$H_k^F(BeV^{3/2})$
16.67	28.98	- 5.74	28.95	- 5.72	28.93	- 5.72
18.05	52.37	7.87	53.23	7.82	53.18	7.84
19.295	245.44	- 9.13	248.08	- 8.87	244.79	- 9.30
20.19	3.73	0.99	3.81	0.93	3.81	0.94
20.67	12.53	4.30	13.66	4.33	13.41	4.39
21.085	81.50	- 1.86	81.84	- 1.78	81.80	- 1.79
22.95	34.52	- 2.32	34.25	- 2.32	34.25	- 2.31
23.44	30.98	3.07	30.92	3.02	30.91	3.02
23.62	61.08	-12.51	60.87	-13.46	57.89	-13.59
24.245	20.59	-18.58	22.68	-17.34	22.63	-18.14
25.62	139.32	70.79	206.62	31.75	204.15	44.15
26.15	- 0.38	0.66	- 5.43	0.58	- 6.22	0.20
26.51	50.88	-30.53	9.32	7.19	84.40	- 3.09
27.18	5.03	2.13	6.40	1.86	6.26	1.93
27.80	53.90	- 6.91	54.88	- 6.58	54.89	- 6.68
28.42	12.98	3.78	12.29	4.12	12.26	4.12
28.73	2.53	0.63	2.20	0.24	2.09	0.26
30.88	21.14	0.59	21.38	0.64	21.33	0.47
31.55	0.84	- 0.80	1.83	- 1.33	1.83	- 1.24
32.07	112.60	- 2.19	114.77	- 0.88	113.70	- 1.31
33.52	78.54	- 7.69	79.81	- 7.29	79.33	- 7.49
44.64	69.72	1.78	70.18	1.76	70.18	1.76
45.04	31.78	- 0.01	30.79	0.61	30.66	0.73
45.78	13.41	3.37	11.36	2.64	11.10	2.61
46.60	16.25	- 1.84	16.64	- 1.87	16.57	- 1.87
51.60	29.18	- 1.53	29.42	- 1.56	29.38	- 1.56
52.22	194.94	0.02	195.47	- 2.18	195.46	0
58.68	86.94	- 4.13	85.55	- 3.83	85.47	- 3.91
60.22	75.47	3.03	74.26	2.71	74.16	2.82
63.80	40.84	2.50	40.73	2.58	40.58	2.51
68.40	7.82	0.27	7.83	0.25	7.80	0.26

than linear in M in Eqs. (38) and (39) does not improve most fission cross-section calculations. It seems likely that for most studies of multilevel interference by the first-order perturbation approach only terms linear in the perturbation need be retained in cross-section expressions.

From Tables III, IV, and V, it appears that the perturbation transformation is surprisingly good. The total cross section parameters are well approximated for all levels and the fission cross section parameters are well approximated for levels other than those near 26 eV. The perturbation transformation predicts qualitatively the effects of interference in nearly all cases.

TABLE V

COMPARISON OF KAPUR-PEIERLS RADIATIVE CAPTURE PARAMETERS IN VARIOUS APPROXIMATIONS FOR 31 LEVELS IN ^{235}U (CRAMÉR DATA)

Level Energy (eV)	POLLA Calculation		PERTA Calculation	
E_k	G_k^γ ($BeV^{3/2}$)	H_k^γ ($BeV^{3/2}$)	G_k^γ ($BeV^{3/2}$)	H_k^γ ($BeV^{3/2}$)
16.67	10.25	-0.03	10.04	-0.01
18.05	11.05	0.01	10.98	0.01
19.295	111.40	-0.08	109.93	-0.01
20.190	2.14	0	1.99	0
20.67	12.77	0.01	12.81	0.01
21.085	102.92	-0.04	102.73	-0.01
22.95	26.88	-0.04	26.84	-0.02
23.44	65.16	0.03	65.00	0.04
23.62	21.52	-0.09	19.65	-0.01
24.245	14.16	-0.17	11.75	-0.09
25.62	7.01	-0.06	6.10	0.51
26 15	0.63	0.26	1.36	0.01
26.51	8.58	-0.02	5.95	-0.43
27.18	1.94	0	1.88	0.02
28.80	21.46	-0.12	20.87	-0.06
28.42	4.62	0.03	4.49	-0.02
28.73	1.40	0.08	1.36	0.07
30.88	30.62	-0.01	30.46	0
31.55	0.93	-0.03	1.81	-0.01
32.07	78.67	0	77.92	0.01
33.52	104.05	-0.04	103.93	0
44.64	11.53	-0.01	11.51	0
45.04	3.36	-0.10	3.28	-0.07
45.78	4.52	0.09	4.34	0.06
46.65	13.50	0	13.45	0
51.60	14.14	0	14.13	0
52.22	18.89	-0.03	18.83	0
58.68	22.31	-0.05	22.24	-0.02
60.22	11.26	0.02	11.18	0.02
63.80	4.51	0	4.76	0
68.40	3.27	0	3.25	0

V. SOME MULTILEVEL INTERFERENCE EFFECTS

The perturbation transformation permits inferences as to the nature of multilevel interference effects, and we briefly note several such inferences.

The range of interference effects is surprisingly long. The interference effects are characterized by the fractional perturbations $M_{cc'}^{kj}$, [Eqs. (19) through (21)], and these vary only as the inverse level spacing for $j = 2$ and as the inverse spacing squared for $j = 1$. Other properties of the fractional perturbations are listed in Sec. II.

The radiative capture cross section usually is observed to have symmetric resonant shapes. This symmetry supposedly arises from the summary of many radiation channels that are incoherent in the sense of Eq. (5). Equations (53) and (54) show that another related property, the constancy of $\Gamma_{k\gamma}(\sum_{c\epsilon\gamma}\Gamma_{kc})$ from level to level, plays a role in diminishing interference.

Finally, we consider briefly the probability distribution of the Kapur-Peierls parameters. Experience has revealed few, if any, deviations from the conjecture of Porter and Thomas[6] that $\Gamma_{kc}^{1/2}$ is distributed as a normal variate with zero mean, that is

$$\Gamma_{kc}^{1/2} = \bar{\Gamma}_{kc}^{1/2} x_{kc} \quad , \tag{57}$$

where $\bar{\Gamma}_{kc}$ is independent of k, and x_{kc} is an independent normal variate with zero mean and unit variance. The similarly successful Wigner distribution for level spacings will be used here only in motivating the assumption that $E_k - E_j$ fluctuates only weakly because of level repulsion.

The total cross section is characterized by the quantities α_k and β_k, and from Eqs. (30), (31), and (57) these are distributed as

$$\alpha_k = \frac{2\pi E}{k_n^2} g_J \bar{\Gamma}_{kn}^{o} x_{kn} \left[x_{kn} + \sum_{k'\neq k} x_{k'n} \frac{(\Gamma_k - \Gamma_{k'})/2}{(E_k - E_{k'})^2 + (\Gamma_k - \Gamma_{k'})/2} \sum_{c'} \Gamma_{kc'} x_{k'c'} x_{kc'}\right] \quad , \tag{58}$$

and

$$\beta_k = \frac{2\pi E}{k_n^2} g_J \bar{\Gamma}_{kn}^{o} x_{kn} \sum_{k'\neq k} x_{k'n} \frac{E_k - E_{k'}}{(E_k - E_{k'})^2 + (\Gamma_k - \Gamma_{k'})^2/4} \sum_{c'} \Gamma_{kc'} x_{k'c'} x_{kc'} \quad . \tag{59}$$

If interference arose from a single channel and a single other level k' then β_k would be distributed as $x_{kn}x_{k'n}x_{kc'}x_{k'c'}$, i.e., as the product of four independent normal variates. If interference arose primarily from a single channel, as in the numerical examples of Sec. IV, than β_k would be distributed as $x_{kn}x_{kc'} \sum_{k'\neq k} x_{k'n}x_{k'c'}a_{k'}$, where the coefficients $a_{k'}$ fluctuate less than do the x_{kc} variates.

We are led to examine variates of the form

$$y_n = x_1 \cdot x_2 \cdot \cdot \cdot x_n \quad , \tag{60}$$

where the variates x_j are independently normal with zero mean and unit variance. The moments of the distributions of these variates are, for $\nu = 1,2,\cdots$,

$$\left\langle y_n^{2\nu-1}\right\rangle = 0 \quad , \tag{61}$$

and

$$\left\langle y_n^{2\nu}\right\rangle = [1 \cdot 3 \cdot 5 \cdot \cdot \cdot (2\nu - 1)]^n \ . \tag{62}$$

A useful distribution shape parameter is the excess of kurtosis, γ_2, defined[21] as

$$\gamma_2 = \frac{\langle y_n^4\rangle}{\langle y_n^2\rangle^2} - 3 \quad , \tag{63}$$

and equal to $3^n - 3$ in this case. A positive value of γ_2 usually means that the distribution is higher near the peak and in the far wings than is a normal ($\gamma_2 = 0$) distribution with the same mean and variance. Equations (61) and (62) permit the computation of moments of all order for noninteger values of n, and although $\sum_{\nu=0}^{\infty} \langle y_b^{2\nu}\rangle/(2\nu)!\ \xi^{2\nu}$ is divergent except at $\xi = 0$, it is reasonable to infer that these moments define a unique probability distribution for positive values of n. Noninteger values of n are useful in approximating the distribution of variates such as $a_1x_1x_2 + a_2x_3x_4$. If $a_1^2 + a_2^2$ is unity, then this variate has zero mean, unit variance, and an excess of kurtosis that varies between 3.25 ($a_1 = a_2$) and 6($a_1 = 1$ or $a_2 = 1$); thus, $a_1x_1x_2 + a_2x_3x_4$ has the same low order moments as has y_n where n varies between about 1.5 and 2.

From Eq. (59) then, we propose that the independent distribution of β_k approximates that of y_n [Eq. (60)], where n is 2 or 3, and that the excess of kurtosis is a useful diagnostic. For the 31 levels in $^{235}U + n$ examined in Sec. IV, the excess of kurtosis in the observed distribution of β_k is 14, a value which corresponds to the variate $y_{2.6}$. A similar result is obtained for the 49 levels assigned by Cramer to the other spin state in $^{235}U + n$.[20] Some of this agreement must be fortuitous in view of the uncertainty in estimating excess of kurtosis from small samples.

Returning to Eqs. (58) and (59), it is seen that the variates α_k and β_k are correlated and for practical application their joint distribution is required. Although the independent distribution of α_k approximates x_{kn} (x_{kn} + constant × y_m), where m is 1 or 2, it is simpler to further approximate the distribution of α_k as x^2_{kn}. In this case, the distribution of the variate $\beta_k/\alpha_k^{1/2}$ approximates y_m, where m is between 1 and 2, and $\beta_k/\alpha_k^{1/2}$ is independent of α_k. Analogous results are obtained for distributions of the other Kapur-Peierls parameters.

The equations developed in this study show that the transformation from Wigner-Eisenbud to Kapur-Peierls formalisms converts a set of (assumed) statistically independent parameters to a set of statistically correlated parameters. The joint distribution of the correlated Kapur-Peierls parameter set is a legitimate object of study as is the independent distribution of a particular parameter. In either case, the experimentalist must recognize that he is sampling from a correlated sample. For example, different results may be obtained if the experimental sample consists of a strongly interfering set of subsets of levels with weak interference between subsets.

APPENDIX A

A LEMMA ON A CLASS OF RATIONAL FUNCTIONS

The rational functions $\sum_{k,k'=1}^{\hat{k}} N_{kk'}/(z-z_k)(z-z^*_{k'})$ and $\sum_{k=1}^{\hat{k}} (A_k+B_kz)/(z-z_k)(z-z^*_k)$ have the same poles of order one when no z_k is real. To determine A_k and B_k in terms of the sets z_k and $N_{kk'}$, the two functions are equal if their residues are equal. Equate residues at the poles z_k and at z^*_k:

$$\frac{A_k + B_k z_k}{z_k - z^*_k} = \sum_{k'=1}^{\hat{k}} \frac{N_{kk'}}{z_k - z^*_{k'}} \quad , \tag{A-1}$$

and

$$\frac{A_k + B_k z^*_k}{z^*_k - z_k} = \sum_{k'=1}^{\hat{k}} \frac{N_{k'k}}{z^*_k - z_{k'}} \quad . \tag{A-2}$$

Solving these equations simultaneously, we have for $k = 1, 2, \cdots, \hat{k}$,

$$A_k = -\sum_{k'=1}^{\hat{k}} \left(N_{kk'} \frac{z^*_k}{z_k - z^*_{k'}} + N_{k'k} \frac{z_k}{z^*_k - z_{k'}} \right) , \tag{A-3}$$

and

$$B_k = \sum_{k'=1}^{\hat{k}} \left(N_{kk'} \frac{1}{z_k - z^*_{k'}} + N_{k'k} \frac{1}{z^*_k - z_{k'}} \right) \quad . \tag{A-4}$$

If, further, $N_{kk'} = N^*_{k'k}$, i.e., the matrix N is self-adjoint, then

$$A_k = -2 \sum_{k'=1}^{\hat{k}} \mathrm{Re} \left(\frac{N_{kk'} z^*_k}{z_k - z^*_{k'}} \right) \quad , \tag{A-5}$$

and

$$B_k = 2 \sum_{k'=1}^{\hat{k}} \mathrm{Re} \left(\frac{N_{kk'}}{z_k - z^*_{k'}} \right) \quad . \tag{A-6}$$

In terms of the real and imaginary parts of $z_k = \mu_k = i\nu_k$,

$$A_k = -2 \sum_{k'=1}^{\hat{k}} \frac{\mathrm{Re}N_{kk'}[\mu_k(\mu_k - \mu_{k'}) - \nu_k(\nu_k + \nu_{k'})] + \mathrm{Im}\, N_{kk'}[\nu_k(\mu_k - \mu_{k'}) + \mu_k(\nu_k + \nu_{k'})]}{(\mu_k - \mu_{k'})^2 + (\nu_k + \nu_{k'})^2} , \quad \text{(A-7)}$$

and

$$B_k = 2 \sum_{k'=1}^{\hat{k}} \frac{\mathrm{Re}N_{kk'}(\mu_k - \mu_{k'}) + \mathrm{Im}N_{kk'}(\nu_k + \nu_{k'})}{(\mu_k - \mu_{k'})^2 + (\nu_k + \nu_{k'})^2} . \quad \text{(A-8)}$$

Some simplification results by observing that

$$A_k = -\mu_k B_k + 2\nu_k \sum_{k'=1}^{\hat{k}} \frac{\mathrm{Re}N_{kk'}(\nu_k + \nu_{k'}) - \mathrm{Im}N_{kk'}(\mu_k - \mu_{k'})}{(\mu_k - \mu_{k'})^2 + (\nu_k + \nu_{k'})^2} . \quad \text{(A-9)}$$

APPENDIX B

PERTURBATION THEORY FOR SYMMETRIC MATRICES

A complex symmetric $N \times N$ matrix B is diagonalized to D by a complex orthogonal $N \times N$ matrix S. Similarly the complex symmetric $N \times N$ matrix $B + \delta B$ is diagonalized to $D + \delta D$ by the complex orthogonal $N \times N$ matrix $S + \delta S$. That is,

$$BS = SZ \quad , \quad \text{(B-1)}$$

and

$$(B + \delta B)(S + \delta S) = (S + \delta S)(D + \delta D) \quad . \quad \text{(B-2)}$$

Subtracting Eq. (B-1) from Eq. (B-2), and ignoring terms of second order in the perturbed quantities,

$$B\delta S + \delta BS = \delta SD + S\delta D \quad . \quad \text{(B-3)}$$

It is convenient to rewrite these equations in terms of the eigenvalues D_{kk} and the eigenvectors s_k, $k = 1, 2, \cdots, N$, column vectors with elements δ_{1k}, $S_{2k}, \cdots, S_{Nk}$. Thus,

$$Bs_k = D_{kk}s_k; \quad k = 1,2,\cdots, N \quad , \quad \text{(B-1}')$$

and

$$B\delta s_k + \delta Bs_k = \delta s_k D_{kk} + s_k \delta D_{kk}; \quad k = 1,2,\cdots, N. \quad \text{(B-3}')$$

Orthogonality of the unperturbed matrix S requires

$$s_k^{tr} s_{k'} = \delta_{kk'}; \quad k, k' = 1,2,\cdots, N \quad . \quad \text{(B-4)}$$

Multiplying Eq. (B-3′) by s_λ^{tr}, one has

$$s_\lambda^{tr} B\delta s_k + s_\lambda^{tr}\delta Bs_k = s_\lambda^{tr}\delta s_k D_{kk} + s_\lambda^{tr} s_k \delta D_{kk};$$
$$\lambda, k = 1,2,\cdots, N \quad ,$$

or, in view of Eq. (B-4),

$$s_\lambda^{tr} B\delta s_k + s_\lambda^{tr}\delta Bs_k = s_\lambda^{tr}\delta s_k D_{kk} + \delta_{\lambda k}\delta D_{kk};$$
$$\lambda, k = 1,2,\cdots, N \quad . \quad \text{(B-5)}$$

Take the transpose of Eq. (B-1′), and recognize that B is symmetric so that $s_k^{tr}B^{tr}$, which is equal to $z_{kk}s_k^{tr}$, is just $s_k^{tr}B$. Thus, rearranging,

$$(D_{\lambda\lambda} - D_{kk})\, s_\lambda^{tr}\delta s_k + s_\lambda^{tr}\delta Bs_k = \delta_{\lambda k}\delta D_{kk};$$
$$\lambda, k = 1,2,\cdots, N. \quad \text{(B-6)}$$

For $\lambda = k$, the perturbation in eigenvalue is determined.

$$\delta D_{kk} = s_k^{tr}\delta Bs_k = \sum_{\lambda,\lambda'=1}^{N} S_{\lambda k}\delta B_{\lambda\lambda'}S_{\lambda' k};$$
$$k = 1,2,\cdots, N \quad . \quad \text{(B-7)}$$

The assumption that B can be diagonalized is equivalent to the assumption that the set s_1, s_2, $\cdots$, s_N is complete, so δs_k can be represented as a linear combination of the s_λ,

$$\delta s_k = \sum_{\lambda'=1}^{N} y_{k\lambda'} s_{\lambda'}, \quad k = 1,2,\cdots, N \quad . \quad \text{(B-8)}$$

Substitute Eq. (B-8) into Eq. (B-6) for the cases $\lambda \neq k$. In view of Eq. (B-4),

$$(D_{\lambda\lambda} - D_{kk})y_{k\lambda} + s_\lambda^{tr}\delta Bs_k = 0; \ \lambda \neq k:$$
$$\lambda, k = 1,2,\cdots, N \quad . \quad \text{(B-9)}$$

Combining Eqs. (B-8) and (B-9),

$$\delta s_k = \sum_{\lambda \neq k} \frac{s_\lambda^{tr}\delta Bs_k}{D_{kk} - D_{\lambda\lambda}} s_\lambda + y_{kk}s_k; \quad k = 1,2,\cdots,N \ . \quad \text{(B-10)}$$

The quantities y_{kk} are as yet undetermined.

Orthogonality of S + δS requires

$$(s_k^{tr} + \delta s_k^{tr})(s_{k'} + \delta s_{k'}) = \delta_{kk'}; \quad k,k' = 1,2,\cdots,N \; . \tag{B-11}$$

Subtract Eq. (B-4) from Eq. (B-11) and linearize, obtaining

$$s_k^{tr}\delta s_{k'} + \delta s_k^{tr} s_{k'} = 0; \quad k,k' = 1,2,\cdots, N \; . \tag{B-12}$$

Substitute Eq. (B-10) into Eq. (B-12), and apply Eq. (B-4),

$$2y_{kk}\delta_{kk'} + (1 - \delta_{kk'})\left[\frac{s_k^{tr}\delta B s_{k'}}{D_{k'k'} - D_{kk}} + \frac{s_{k'}^{tr}\delta B s_k}{D_{kk} - D_{k'k'}}\right] = 0;$$

$$k,k' = 1,2,\cdots, N \; . \tag{B-13}$$

In view of the symmetry of δB one obtains, for $k,k' = 1,2,\cdots, N$,

$$s_k^{tr}\delta B s_{k'} = \sum_{\lambda,\lambda'} S_{\lambda k}\delta B_{\lambda\lambda'} S_{\lambda' k'} = \sum_{\lambda,\lambda'} S_{\lambda' k'}\delta B_{\lambda'\lambda} S_{\lambda k} =$$

$$s_{k'}^{tr}\delta B s_k \quad , \tag{B-14}$$

so the square bracket in Eq. (B-13) is identically zero. Thus, to preserve orthogonality of S + δS (to first order in the perturbation), it is necessary to set y_{kk} equal to zero. Finally, Eq. (B-10) becomes

$$\delta s_{jk} = \sum_{\substack{\lambda \neq k \\ \lambda,k=1}}^{N} \frac{\sum_{\lambda',\lambda''=1}^{N} S_{\lambda'\lambda}\delta B_{\lambda'\lambda''} S_{\lambda'' k}}{D_{kk} - D_{kk}} \, s_{j\lambda};$$

$$j,k = 1,2,\cdots, N. \tag{B-15}$$

APPENDIX C

INPUT AND OUTPUT FOR THE PERTA PROGRAM

Input

Card 1: Any 80 column alphanumeric title.

Card 2: 16I5 format.

MØRE: Positive if there are more cases in this job.

NL: Number of interfering levels.

NF: Number of fission channels.

NNLIN: Equals 1 if $R_{nn}^{kj} = M_{nn}^{kj}$.
Equals 0 if Eqs. (24) and (25) are used for R_{nn}^{kj}.

NFLIN: Equals 1 if Eqs. (40) and (41) are used for $Q_{cc'}^{kk',j}$.
Equals 0 if Eqs. (39) and (40) are used for $Q_{cc'}^{kk',j}$.

Card 3: 8E10.3 format.

ANUC: Target nuclear mass in AMU.

Card 4: 8E10.3 format. Wigner-Eisenbud parameters.
Level energy for level 1.
Statistical weight factor for level 1.
Reduced neutron width for level 1
Radiative capture width for level 1.
Partial fission widths for level 1 for fission channels 1,···, NF.

Cards 5 to 4 + NL: 8E10.3 format. Wigner-Eisenbud parameters for remaining levels.

Output

The input Wigner-Eisenbud parameters are edited together with the total level widths. The remaining edits are listed in Sec. III. Definitions of program variables, which label some edits, are listed on comment cards early in the program deck.

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