

Statistical significance of spreading widths for doorway states

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(Received 7 February 1979)

The strength function constructed as the Lorentz-weighted average of the reduced widths of the Wigner-Eisenbud R matrix (or of a reactance K matrix) is a continuous and well-defined function of energy for a fragmented doorway state (isobaric analog resonance, fission isomer, etc.) in both weak and strong coupling. If the half-width I of the Lorentz weighting function is chosen appropriately, this strength function itself approximates a Lorentzian whose width is the spreading width Γ_j^\dagger of Feshbach, Kerman, and Lemmer. An ensemble of 400 doorway systems characterized by coupling strengths ranging from strong to weak is used to study properties of Γ_j^\dagger and to determine the accuracy with which it can be determined for a particular doorway by a least-squares fit to the strength function. The results of this numerical study show that (1) Γ_j^\dagger is a characteristic of each doorway state system, and that (2) its value can be determined from experimentally measured resonance energies and widths with an uncertainty which is less than the fluctuations in its value from one system to another and which decreases as the coupling strength decreases.

[NUCLEAR REACTIONS spreading of doorway states, fine structure, isobaric analog states.]

I. INTRODUCTION

The fragmentation of a doorway state¹ by a residual interaction which breaks a symmetry of the model Hamiltonian produces a distribution of its strength among neighboring states recognizable by the approximately Lorentzian envelope of reduced partial widths.²⁻⁴ The envelope may display some asymmetry if the states responsible for the fine structure have some "intrinsic" transition strength of their own. The width of this envelope measures the strength of the symmetry-breaking interaction. The isobaric analog states (IAS) provide examples of considerable interest because the spreading is produced by interactions which violate charge symmetry. The possibility of extracting reliable information on symmetry-breaking interactions places a high premium on a reliable means for determining a spreading width which is precisely and unambiguously related to the matrix elements of the symmetry-breaking interaction. Unfortunately much of the literature on this subject is flawed by (1) confusion between different parameters for measuring the transition strength of a state,⁵ and/or (2) failure to recognize the significance of different averaging procedures used to obtain a smooth (or discontinuous) function to represent the distribution of strength.⁶

This paper reports an investigation of a straightforward method for using the reduced partial widths from a multilevel (Wigner-Eisenbud) R -matrix analysis of differential cross sections to determine a spreading width Γ_j^\dagger which is a Lorentzian average of the symmetry-breaking matrix

elements to the doorway state.¹ The method consists of doing a least-squares fit to a strength function (SF) which is a Lorentz-weighted average of these widths.^{3,4} The only previous application of the method has been made by Di Toro,⁷ who used it to analyze the fine structure associated with several isobaric analog states (IAS). The accuracy of the procedure and the significance of the spreading width have been studied by applying it to four ensembles of 400 fine-structure (FS) patterns each constructed by drawing level spacings from a Wigner distribution and coupling matrix elements from a normal distribution. The results show that

(1) a Lorentzian average of the symmetry-breaking matrix elements to a *particular* doorway state can be determined with an accuracy of better than 10% for both "weak coupling" ($\Gamma^\dagger \lesssim \langle D \rangle$) and "strong coupling" ($\Gamma^\dagger \gg \langle D \rangle$), and

(2) each spreading width Γ_j^\dagger characterizes one particular doorway system with its set (M_i) of coupling matrix elements to FS states at energies (ϵ_i).

These conclusions differ from those of Lane, Lynn, and Moses (LLM) who also analyzed four ensembles, each with 100 fine-structure patterns for doorway states, which were based on the same model as that used in the present study.⁸ A careful reading of their paper reveals, however, that their results related to the determination of an *ensemble average* of a spreading parameter $W_1 = 2\pi \langle M_i^2 \rangle / \langle D_i \rangle$ and to the determination of its *standard deviation* for the *ensemble*. The present study will show that W_1 does indeed fluctuate con-

siderably from one doorway system to another (although the variances of LLM appear to be in error by a factor of 2). However, this has no bearing on the accuracy with which the doorway spreading width Γ_I^\dagger of Feshbach, Kerman, and Lemmer¹ can be determined from the R -matrix parameters ($E_\lambda, \gamma_{\lambda c}^2$) of the microresonances in the fine-structure pattern.

II. STRENGTH FUNCTION FOR DOORWAY STATES

A. (MMKP) strength function

Experimental measurements of differential cross sections with good energy resolution have usually been analyzed using the multilevel R matrix of Wigner-Eisenbud to obtain the resonance energies E_λ and reduced partial widths $\gamma_{\lambda c}$.⁹

As shown by MacDonald and Mekjian,³ and independently by Kerman and de Toledo Piza,⁴ the Lorentz-weighted strength function (SF) of the reduced widths

$$S(E, I) = \frac{I}{\pi} \sum_{\lambda} \frac{\gamma_{\lambda c}^2}{(E - E_\lambda)^2 + I^2} \quad (1)$$

can be used to extract both the properties of the underlying doorway state and the Lorentz-weighted average of the squared matrix elements of the symmetry-breaking or residual interaction to fine-structure (FS) states. In the simple case of coupling of a doorway state at energy E_D of reduced width γ_{Dc} to FS states which have zero intrinsic widths, the SF is also given identically by

$$S(E; I) = \frac{\gamma_{Dc}^2 \Gamma_S / 2\pi}{(E - \bar{E}_D)^2 + (\Gamma_S / 2)^2} \quad (2)$$

with an energy-dependent shift and width.^{3,4} The width is given by $\Gamma_S = \Gamma_I^\dagger + 2I$ with

$$\Gamma_I^\dagger(E) = 2I \sum_i \frac{M_i^2}{(E - \epsilon_i)^2 + I^2}, \quad (3)$$

and the doorway energy is $\bar{E}_D \equiv E_D + \Delta_I(E)$, where

$$\Delta_I(E) \equiv \sum_i \frac{(E - \epsilon_i) M_i^2}{(E - \epsilon_i)^2 + I^2}. \quad (4)$$

The SF defined by these equations, the MMKP strength function, has several important properties, not shared by other SF defined in discussions of fine structure associated with doorway states,³⁻¹⁰ which are discussed in the following subsections.

B. Strength distribution

Equations (1) and (2) give the distribution of strength measured by reduced widths of the Wigner-Eisenbud R matrix (or corresponding quantities for the K matrix). It can therefore be con-

structed from experimentally determined ($E_\lambda, \gamma_{\lambda c}^2$). LLM prefer to work with the intensity $|\langle \Psi | \hat{z} \rangle|^2$ of the FS state $|\hat{z}\rangle$ present in the exact R -matrix state $|\Psi\rangle$ instead of $\gamma_{\lambda c}^2$. Unfortunately, in the general case of spreading to FS states with intrinsic decay widths, these intensities cannot be deduced from the experimental data. Therefore, in general the LLM-SF cannot be constructed from experimentally determined quantities, and it is only of theoretical interest. For the case of FS states with no intrinsic widths, studied in their paper, $\gamma_{\lambda c}^2 = \gamma_{Dc}^2 |\langle \Psi | \hat{z} \rangle|^2$, and the intensities are proportional to the reduced widths.

It should be noted that both the MMKP-SF and that of LLM differ from the SF defined by Lane in his analysis, "line broadening of unbound states."¹⁰ In this section of his review Lane uses the term " R matrix" to refer to the Kapur-Peierls representation of the S matrix, which uses states with complex boundary conditions and complex eigenvalues, rather than to the Wigner-Eisenbud (WE) R matrix, which uses states with standing-wave boundary conditions. His SF for unbound states relates to complex poles and complex residues of the S matrix rather than to the real resonance energies and real reduced widths of the WE R matrix. For a fragmented doorway state the energy dependence of the S -matrix widths is *qualitatively* different from that of the WE reduced widths.² For example, the distribution of WE reduced widths is *independent* of the decay width Γ^\dagger of the doorway state, whereas the S -matrix widths follow a non-Lorentzian envelope with a "width" equal to $\Gamma^\dagger + \Gamma^\dagger$. From a practical viewpoint, the Kapur-Peierls representation is useless for the analysis of high resolution data on fine structure both because the reduced widths and energies are complex, and because they are dependent and must satisfy complicated unitarity constraints.¹¹ Therefore, high resolution experiments on doorways are analyzed using multilevel WE R -matrix theory; the discussion of line-broadening for unbound states in this review article is therefore not applicable to the ($\gamma_{\lambda c}^2, E_\lambda$) obtained from such analyses.

C. Parametric form of MMKP-SF for fragmented doorway states

The parameter dependence of the MMKP-SF can be rigorously established. The MMKP-SF for a fragmented doorway state is given by Eq. (2), but it is also *identically equal* to the *general form* of the MMKP-SF given by Eq. (1) for *any* averaging width I and *any* strength for the average coupling matrix element. Equation (2) shows directly that the MMKP-SF for a fragmented doorway approximates a Lorentzian when I is increased to a value

become nearly constant over an energy interval centered near the doorway. When this occurs $\Gamma_i^{\dagger}(E_D)$ becomes a parameter characterizing the coupling of the doorway to the FS states, and its value is precisely defined by Eq. (3) as a Lorentz average of the coupling matrix elements. Since Eq. (2) is identically equal to Eq. (1), it can be used to calculate the MMKP-SF directly from the microscopic parameters (M_i, ϵ_i) . Since this route leads through $\Gamma_i^{\dagger}(E)$ and $\Delta_i(E)$, it is also ideally suited to the model study of this report.

It should be noted that the SF defined by LIM as the sliding box average of $\gamma_{\lambda c}^2$ or of $|\langle \Psi | i \rangle|^2$ is a histogram. In weak coupling it never approximates a well-defined smooth curve even for large averaging intervals. In *very* strong coupling their SF does define a smooth curve, but this curve is *not* Lorentzian. Instead, their SF follows the arc-tangent of a Lorentzian,⁶ a fact well known to experimentalists who measure resonant excitation functions with detectors of finite resolution.¹²

D. Continuity of the MMKP-SF

This SF given by Eq. (1) is a *continuous* function of energy which can be calculated directly from the reduced widths of a multilevel (Wigner-Eisenbud) R -matrix fit to high resolution data. The continuity of the SF is essential to determining the spreading width Γ_i^{\dagger} of a doorway directly from the resonance parameters $(\gamma_{\lambda c}^2, E_{\lambda})$ by performing a least-squares fit to the parametric form. By contrast, the study by Lane, Lynn, and Moses used a discontinuous summed strength function which was fitted to the (continuous) integral of the Lorentzian of Eq. (2). The fitting procedure is necessarily ill defined and for intermediate to weak coupling (as in most IAS) meaningless. LLM removed this ambiguity of the fitting procedure by arbitrarily selecting the midpoints of the steps in the histogram of the summed strength as the fitting points. However, there is no reason to expect the spreading width obtained from such a fit to be significant when the coupling is weak.

III. STRENGTH FUNCTION ANALYSIS OF FRAGMENTED DOORWAY STATES

A. Model for fragmented doorway states

The results presented in this paper are based on the application of Eqs. (2), (3), (4) to ensembles of fine-structure patterns. Each ensemble contained 100 fine-structure patterns. Each fine-structure pattern in a given ensemble was constructed by drawing level spacings D_i for fine-structure states from a Wigner distribution¹³ and matrix elements M_i from these states to a doorway

from a normal distribution with zero mean. The entire study was carried out in *dimensionless units* obtained by taking the *unit of energy* to be the *average level spacing* for the Wigner level spacing distribution. In these units the spacing distribution is

$$P_L(D) = \frac{1}{2}\pi D \exp(-\pi D^2/4), \quad (5)$$

and the matrix elements were drawn from

$$P_C(M) = (2\pi\langle M^2 \rangle)^{-1/2} \exp(-M^2/2\langle M^2 \rangle). \quad (6)$$

Note that with this choice of dimensionless units $\langle D \rangle = 1$.

Each *ensemble* of 100 fine-structure patterns is characterized by a given value of $\langle M^2 \rangle$, which completely determines the distribution functions from which are drawn the matrix elements for every fine-structure pattern in that ensemble. Choosing this parameter means choosing a value for $W = 2\pi\langle M^2 \rangle / \langle D \rangle = 2\pi\langle M^2 \rangle$. The level spacings and matrix elements for a fine-structure pattern in that ensemble are then found by solving the equations

$$\int_0^{D_i} dD P_L(D) = u_{2i-1}, \quad i = 1, 2, \dots, 100 \quad (7)$$

$$\int_{-\infty}^{M_i} dM P_C(M) = u_{2i},$$

where (u_i) is a set of 200 random numbers on the unit interval. The equation for the matrix elements can be written

$$\text{erf}(m_i) = u_{2i}, \quad i = 1, 2, \dots, 100 \quad (8)$$

with the normalized error function

$$\text{erf}(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x dy e^{-y^2/2}, \quad (9)$$

and the variable $m_i \equiv M_i / \langle M^2 \rangle^{1/2}$. Since the (m_i) depend only on the set of random numbers, the dimensionless matrix elements are simply proportional to W .

$$M_i = \langle M^2 \rangle^{1/2} m_i$$

$$= m_i (W/2\pi)^{1/2}, \quad i = 1, 2, \dots, 100. \quad (10)$$

In the present study 100 sets (u_i) of 200 random numbers each were used to generate the 100 sets of level spacings (D_i) and 100 sets of matrix parameters (m_i) . The energies (ϵ_i) of the FS states and the coupling matrix elements M_i for each doorway system in a given ensemble then were calculated from one set of (u_i) and one set of $\{m_i\}$ through Eq. (10) and

$$\epsilon_i = 150 + \sum_{j=1}^i D_j, \quad i = 1, \dots, 100. \quad (11)$$

Since $\langle D_i \rangle \cong 1$ within a 5% sample deviation, the $\{\epsilon_i\}$ span the energy range $E = 150-250$. To reduce

effects due to the finite number of levels, the location of the doorway was always chosen to be $E_D = 200$, the approximate center of the pattern.

The results of the model study can easily be related to isobaric analog resonances by noting that the average level spacing for the fine-structure patterns in the survey of Bilpuch *et al.*⁹ is $\langle D \rangle \sim 10$ keV. The IAS in this survey are located around 2000 keV. Therefore, the dimensionless energies of the model study can be scaled approximately by a factor of 10 to compare with the IAS.

B. Determination of spreading widths by least-squares fitting

The MMKP-SF of Eq. (1) for a fragmented doorway state approximates a Lorentzian if there is some averaging width I for which the shift $\Delta_I(E)$ and $\Gamma_I^{\dagger}(E)$ and nearly constant over the energy interval $\bar{E}_D - \Gamma_S/2 < E < \bar{E}_D + \Gamma_S/2$. The parameters \bar{E}_D and Γ_S can be determined by performing a least-squares fit of Eq. (2) to Eq. (1), taking \bar{E}_D and Γ_S as constants to be determined. If this can be done with sufficient accuracy, the spreading width $\Gamma_I^{\dagger}(\bar{E}_D) = \Gamma_S - 2I$ is then determined. The fractional error in Γ_S arises from fluctuations in $\Delta_I(E)$ and $\Gamma_I^{\dagger}(E)$. Increasing I will reduce the fluctuations and hence reduce the error in Γ_S . But since the fractional error in Γ_I^{\dagger} is $\Delta\Gamma_I^{\dagger}/\Gamma_I^{\dagger} = (\Delta\Gamma_S/\Gamma_S)(\Gamma_S/\Gamma_I^{\dagger})$, it is profitable to use the smallest values of I possible, i.e., $I \sim \Gamma_I^{\dagger}$.

In this model study the microscopic parameters (M_i, ϵ_i) can be used to calculate the energy-dependent quantities $\bar{E}_D(E)$ and $\Gamma_S(E)$. The SF can be calculated, therefore, by using Eq. (2) with these energy-dependent quantities as an identical representation of Eq. (1). Thus, Eq. (2) with *constant* values for \bar{E}_D and Γ_S is fitted to Eq. (2) with energy-dependent *functions* for \bar{E}_D and Γ_S . The fitted values for \bar{E}_D and Γ_I^{\dagger} can then be compared with the exact values $\bar{E}_D(\bar{E}_D)$ and $\Gamma_I^{\dagger}(\bar{E}_D)$ in order to ascertain the accuracy of the fitting procedure. Since γ_{Dc}^2 is simply an amplitude factor which has no effect on either the width of the maximum in the SF or upon the fitting procedure, it was set equal to unity in all the calculations of this paper.

The least-squares LSQ fitting was performed by the program VAO5A written by M. J. D. Powell

for the Harwell Subroutine Library. This program has been thoroughly tested in a variety of conditions and found to be extremely fast and reliable.

IV. RESULTS

Ensemble averages of a number of different spreading parameters and their standard deviations are presented in the tables together with the predictions derived in the Appendix using various moments of the distribution functions of Eqs. (5) and (6). All averages over the levels of a particular doorway system are denoted by angular brackets; curly brackets are used to denote averages over an ensemble defined by an assigned value for $W = 2\pi\langle M^2 \rangle / \langle D \rangle$. In the following subsections the ensemble averages of spreading parameters and the results of the least-squares (LSQ) fitting are discussed in detail.

A. Ensemble averages of W_1 and W_2

In the literature, discussions of SF frequently do not distinguish between several quantities which measure the strength of the coupling of the doorway state to FS states. Generally, $2\pi\langle M^2 \rangle / \langle D \rangle$, $2\pi\langle M^2/D \rangle$, and Γ_I^{\dagger} are assumed to be equal. To test this assumption, as well as to determine the variation in these quantities from one system to another in a given ensemble, values of $W_1 \equiv 2\pi\langle M_i^2 \rangle / \langle D_i \rangle$ and $W_2 \equiv 2\pi\langle M_i^2/D_i \rangle$ were calculated for each of 100 systems in the ensemble characterized by $W \equiv 2\pi\langle M^2 \rangle = 2\pi\langle M^2 \rangle / \langle D \rangle = 2\pi$. The ensemble averages and variances of these quantities are displayed in Table I.

In agreement with Eq. (A3) of the Appendix, the ensemble average $\{W_1\}$ is equal to the ensemble parameter W within the statistical error $\sigma/\sqrt{100}$ for an ensemble of 100 systems. Moreover, the standard deviation $\sigma = 0.97$ for the distribution of values for W_1 in the ensemble is in good agreement with the value $\sigma = 0.95$ predicted by Eq. (A9) for the case of 100 levels per system. The ensemble average $\{W_2\} = 9.87$ also agrees satisfactorily with the value of $\{W_2\} = 9.56$ predicted by Eq. (A11) for an ensemble with $W = 2\pi$. The statistical error of $\{W_2\}$ is much larger than that for $\{W_1\}$, although it is, of course, not infinite as for an in-

TABLE I. Ensemble averages of spreading parameters.

Parameter	$W = 2\pi \langle M^2 \rangle / \langle D \rangle = 6.2832$		
	Ensemble average	Standard deviation	Statistical error in ensemble average
W_1	6.16	0.97	0.10
LLM	6.56	2.02	0.20
W_2	9.56	2.42	0.24

TABLE II. Ensemble average of $\langle \Gamma_I^\dagger(E) \rangle$.

I	0.5	1.0	1.5	2.0	2.5	3.0
$\langle \Gamma_I^\dagger(E) \rangle$	6.17	6.13	6.08	6.04	5.99	5.95
	6.217 ^a	6.215 ^a	6.215 ^a	6.214 ^a	6.212 ^a	6.210 ^a
	± 1.27	± 1.23	± 1.20	± 1.18	± 1.15	± 1.13

^a With finite interval corrections.

finite ensemble. However, the value of σ for the distribution of W_2 values is $\sigma = 5.88$, compared to $\{W_2\} = 9.56$.

The values in Table I labelled LLM are taken from Table I of the paper by Lane, Lynn, and Moses.⁸ Their value for the standard deviation differs by about a factor of 2 from the value predicted by Eq.(A9) for this ensemble.

B. Averages of the spreading width Γ_I^\dagger

Ensemble average of $\langle \Gamma_I^\dagger \rangle$

The spreading width Γ_I^\dagger defined by Eq. (3) fluctuates with energy so that a comparison with spreading parameters W , W_1 , and W_2 must be made by averaging Γ_I^\dagger over an energy interval chosen to minimize end effects due to the finite number of FS states. The coupling matrix elements for a physical doorway state, e.g., an IAS, undoubtedly extend over several hundred levels, whereas the model contains only 100 states. Therefore, $\langle \Gamma_I^\dagger \rangle$ was obtained by averaging over the energy interval $175 \leq E \leq 225$. From these average values for each doorway the ensemble average $\langle \Gamma_I^\dagger \rangle$ and the standard deviation

$$\sigma(\langle \Gamma_I^\dagger \rangle) \equiv \{ \langle \Gamma_I^\dagger \rangle - \langle \Gamma_I^\dagger \rangle^2 \}^{1/2}$$

were calculated for the ensemble $W = 2\pi$. These quantities are presented in Table II.

In agreement with the prediction of Eq. (A18) the ensemble average of $\langle \Gamma_I^\dagger \rangle$ is close to the value of the spreading parameter W and to the ensemble average $\{W_1\}$; it does not approximate $\{W_2\} = \{2\pi \langle M_i^2 / D_i \rangle\}$. This is interesting because the usual approximation of replacing the sum in Eq. (3) by an integral gives W_2 . The fractional en-

semble standard deviation of $\langle \Gamma_I^\dagger \rangle$ is approximately 0.20 and independent of I . The fractional standard deviation predicted by Eq. (A19) is approximately 0.15.

The decrease of $\langle \Gamma_I^\dagger \rangle$ with increasing I suggests the effect of the finite number of levels. A correction can be calculated from the picket fence model in which there are an infinite number of equally spaced states coupled to the doorway by a constant matrix element, M^2 .¹⁴ The model is somewhat unrealistic because it implies an infinite value for the expectation value $\langle D | V^2 | D \rangle$ of the square of the effective nucleon-nucleon interaction. Thus the correction will be *overestimated*. The contribution $\Delta \Gamma_I^\dagger$ of states *outside* the energy range of $E_s \leq E \leq E_F$ is given approximately as

$$\Delta \hat{\Gamma}_I^\dagger(E) \approx \frac{2\pi \langle M^2 \rangle}{\langle D \rangle^2} \left[1 - \frac{1}{\pi} \left(\tan^{-1} \frac{E_F - E}{I} + \tan^{-1} \frac{E - E_s}{I} \right) \right]. \quad (12)$$

In Table I the values of $\langle \Gamma_I^\dagger \rangle$ are also given with this correction included. The corrections are small but sufficient to remove the dependence on I . The corrected values $\langle \Gamma_I^\dagger \rangle = 6.21-6.22$ differ from $W = 6.28$ by about 1%, less than the statistical error for the ensemble of $0.15/\sqrt{100}$

rms fluctuations of Γ_I^\dagger with energy

The spreading width $\Gamma_I^\dagger(E)$ fluctuates with energy, although increasing I decreases the magnitude of these fluctuations. The fluctuations in Γ_I^\dagger will be reflected in an uncertainty in the least-squares fitted value for Γ_s . Therefore, it is useful to calculate the variance of $\Gamma_I^\dagger(E)$ in the system, i.e., $\sigma^2(\langle \Gamma_I^\dagger \rangle) \equiv \langle (\Gamma_I^\dagger - \langle \Gamma_I^\dagger \rangle)^2 \rangle$. Of course, the value of this

TABLE III. Fluctuations in spreading width with energy.

I	0.5	1.0	1.5	2.0	2.5	3.0
$\langle \Gamma_I^\dagger \rangle$	6.217 ^a	6.215 ^a	6.214 ^a	6.214 ^a	6.212 ^a	6.210 ^a
$\sigma_{\Gamma_I^\dagger} / \langle \Gamma_I^\dagger \rangle$	0.84	0.56	0.44	0.37	0.32	0.29
$1/\sqrt{\pi I}$	0.80	0.56	0.46	0.40	0.36	0.33

^a With finite interval correction.

quantity will be different for every doorway system in a given ensemble, so it is averaged over the ensemble $W=2\pi$, and the result is given in Table III. The fractional standard deviation of these energy fluctuations in Γ_I^\dagger is independent of the ensemble, as explained in Sec. III A. This is also the fractional rms fluctuation.

The fluctuations of $\Gamma_I^\dagger(E)$ with energy are largest for small I and decrease as this averaging is increased. The fractional rms fluctuation for the ensemble follows very closely the theoretical expression $1/(\pi I)^{1/2}$ given by Eq. (A21). However, even for an averaging interval of $I=3$, the fractional standard deviation is nearly 30%. Thus the value of $\Gamma_I^\dagger(E)$ is by no means constant as a function of energy over the interval $175 \leq E \leq 225$.

Therefore, the value of the spreading width at the location of the doorway E_D is a local quantity which does not approximate the average value of Γ_I^\dagger ; it depends on the particular set of (M_i, ϵ_i) and on the location of the doorway.

Fluctuations in $\Gamma_I^\dagger(E_D)$

Already we have seen that the value of $\Gamma_I^\dagger(E_D)$ for a particular fragmented doorway will depend on the location of the doorway as much as on the set (M_i, ϵ_i) . This can be verified by calculating the ensemble average $\{\Gamma_I^\dagger(E_D)\}$ and the ensemble fractional standard deviation. These quantities are presented in Table IV. The fluctuations in $\Gamma_I^\dagger(E_D)$ from one doorway system to another show a decrease with increasing I . According to Eq. (A16) the fractional standard deviation is nearly equal to $1/\sqrt{\pi I}$. The relatively large fractional standard deviation of nearly 25% even for $I=6$ shows that $\Gamma_I^\dagger(E_D)$ for a particular doorway can and does deviate considerably from the ensemble average value.

C. Least-squares fitted values for Γ_I^\dagger

The least-squares (LSQ) fitting procedure described in III B was applied to each of 100 systems in four different ensembles characterized by $W/2\pi = 0.5, 0.25, 0.10, \text{ and } 0.025$. Furthermore, the LSQ

TABLE V. $\Gamma_I^\dagger(E_D)$ from least-squares fit to strength function.

\hat{I}	1.0	2.0	3.0	4.0
$W=3.14$				
$\{\hat{\Gamma}_I^\dagger(E_D)\}$	3.03	2.97	2.94	2.92
$\{\hat{\Gamma}_{\text{FIT}}\}$	2.74	2.90	2.91	2.90
$\sigma_{\text{FIT}}/\{\Gamma_{\text{FIT}}\}$	± 0.31	± 0.16	± 0.10	± 0.07
$W=1.57$				
$\{\hat{\Gamma}_I^\dagger(E_D)\}$	1.52	1.48	1.47	1.46
$\{\hat{\Gamma}_{\text{FIT}}\}$	1.41	1.46	1.47	1.46
$\sigma_{\text{FIT}}/\{\Gamma_{\text{FIT}}\}$	± 0.22	± 0.12	± 0.08	± 0.06
$W=0.628$				
$\{\hat{\Gamma}_I^\dagger(E_D)\}$	0.607	0.594	0.589	0.583
$\{\hat{\Gamma}_{\text{FIT}}\}$	0.582	0.590	0.589	0.584
$\sigma_{\text{FIT}}/\{\Gamma_{\text{FIT}}\}$	± 0.15	± 0.10	± 0.07	± 0.06
$W=0.157$				
$\{\hat{\Gamma}_I^\dagger(E_D)\}$	0.152	0.148	0.147	0.146
$\{\hat{\Gamma}_{\text{FIT}}\}$	0.147	0.148	0.148	0.146
$\sigma_{\text{FIT}}/\{\Gamma_{\text{FIT}}\}$	± 0.11	± 0.08	± 0.06	± 0.04

fit was performed on each doorway system for four different values of the averaging width, $I=1, 2, 3, \text{ and } 4$. Therefore, the accuracy of the LSQ determination of $\Gamma_I^\dagger(E_D)$ was tested for systems in ensembles characterized by values of the spreading parameter ranging from weak to intermediate coupling. The sensitivity of the method to fluctuations in $\Gamma_I^\dagger(E)$ is measured by the accuracy of the determination of $\Gamma_I^\dagger(E_D)$ for various values of the averaging width I . Table V summarizes the results of the LSQ fitting procedure for all 1600 = $4 \times 4 \times 100$ cases. Ensemble average values $\{\Gamma_{\text{FIT}}\}$ are presented for comparison with the en-

TABLE IV. Ensemble average of spreading width $\Gamma_I^\dagger(E_D)$.

I	$W=6.28 (=2\pi \langle M^2 \rangle / \langle D \rangle)$					
	1.0	2.0	3.0	4.0	5.0	6.0
$\{\Gamma_I^\dagger(E_D)\}$	6.06	5.94	5.89	5.83	5.77	5.70
	6.15 ^a	6.10 ^a	6.13 ^a	6.15 ^a	6.17 ^a	6.18 ^a
$\sigma/\{\Gamma_I^\dagger(E_D)\}$	± 0.54	± 0.40	± 0.34	± 0.31	± 0.28	± 0.26
$1/\sqrt{\pi I}$	0.56	0.40	0.33	0.28	0.25	0.23

^a Finite interval correction included.

semble average of the calculated values of $\{\Gamma_I^\dagger(E_D)\}$. The error in the determination of $\Gamma_I^\dagger(E_D)$ is measured by the fractional standard deviation for each I in each ensemble, i.e., by

$$\sigma_{\Gamma_{\text{FIT}}}/\{\Gamma_{\text{FIT}}\} = \frac{\{[\Gamma_{\text{FIT}} - \Gamma_I^\dagger(E_D)]^2\}^{1/2}}{\{\Gamma_{\text{FIT}}\}}. \quad (13)$$

The significance of the results presented in Table V can be seen by comparison with the ensemble averages and fractional standard deviations shown in Tables I–IV. Note first that the uncertainty in the ensemble average value $\{\Gamma_I^\dagger(E_D)\}$ determined by the LSQ fitting procedure is given by $\sigma/\sqrt{100}$ where the best value for σ is the sample standard deviation, $\sigma = \sigma_{\Gamma_{\text{FIT}}}$. For approximately $\frac{1}{3}$ of the 16 cases the difference between the two averages $\{\Gamma_I^\dagger(E_D)\}$ and $\{\Gamma_{\text{FIT}}\}$ exceeds the statistical uncertainty, as one expects for normally distributed errors. This was confirmed by a histogram of the errors $[\Gamma_{\text{FIT}} - \Gamma_I^\dagger(E_D)]$ for the ensemble $W = \pi$ which was constructed and found to be very close to a normal distribution.

The uncertainty in the value of $\Gamma_I(E_D)$ obtained by an LSQ fit to the SF for a *particular* doorway system is approximately $\sigma_{\Gamma_{\text{FIT}}}$. A comparison with Tables II and IV reveals that this uncertainty is always less than the fractional standard deviation in the average values $\{\langle\Gamma_I^\dagger\rangle\}$ and $\{\Gamma_I^\dagger(E_D)\}$. Moreover, the fractional standard deviations in these quantities are independent of the ensemble spreading parameter W , whereas the fractional uncertainty $\sigma_{\Gamma_{\text{FIT}}}/\Gamma_{\text{FIT}}$ decreases with decreasing W . Both observations are consistent with the fact that the LSQ fitting determines $\Gamma_I^\dagger(E_D)$, a quantity which characterizes a particular doorway state and not an ensemble parameter.

The uncertainties in the LSQ fitting procedure arise mostly from the fluctuations in $\Gamma_I^\dagger(E)$, which cause the doorway SF to deviate from a Lorentzian. However, fluctuations in $\Gamma_I^\dagger(E)$ are important only if they occur over the maximum of the SF. Now the *width* of the maximum of the SF is minimally Γ_I^\dagger , which Eq. (10) shows to be proportional to the ensemble spreading parameter W . On the other hand, the *widths of the fluctuations* in Γ_I^\dagger are quite independent of W , being entirely determined by the properties of the dimensionless distributions of Eqs. (8) and (9). Therefore, as W decreases so also do the fluctuations in $\Gamma_I^\dagger(E)$ over the maximum in the SF. The SF more closely approximates a Lorentzian, and the value of $\Gamma_I^\dagger(E_D)$ is more accurately determined by the LSQ fitting procedure. Thus, $\Gamma_I^\dagger(E_D)$ is determined with increasing accuracy by the fitting procedure as the coupling becomes weaker.

V. COMPARISON WITH LLM

The results of LLM have been quoted by Bilpuch *et al.*⁹ as establishing that spreading widths of IAS can generally not be determined with a statistical error of less than 30–40%. Since this assertion is apparently contradicted by the results presented in Table V, the work of LLM must be re-evaluated. The following discussion (1) reviews the concept of an ensemble SF introduced by LLM, (2) assesses its relevancy for the analysis of line broadening, and (3) relates the numerical results of LLM to those in this paper.

A. Ensemble strength function of LLM

The SF formed by doing a sliding box average of $\gamma_{\lambda c}^2$ is a histogram, and in the case of weak coupling it is meaningless to speak of its spreading width. Recognition of this fact led LLM to propose that every physical doorway system be considered as belonging to fictitious ensemble of systems. The squared matrix elements of the ensemble have some average value $\langle M^2 \rangle$ and the level spacing is also fixed, but the LLM did not specify the respective distribution functions. LLM then considered the ensemble distribution function constructed by box averaging the *totality* of $\gamma_{\lambda c}^2$ for all the systems in the ensemble, and conjecture that it is of the form

$$\tilde{S}(E) = \frac{W/2\pi}{(E - E_D)^2 + (W/2)^2}, \quad (14)$$

where $W = 2\pi\langle M^2 \rangle / \langle D \rangle$.

B. Irrelevancy of the ensemble strength function

The ensemble of LLM contains only one physical doorway system with its set of (M_i, ϵ_i) generating the observed $(E_\lambda, \gamma_{\lambda c}^2)$. In fact, the entire ensemble must be constructed using only the information that can be inferred from the set of experimentally determined $(E_\lambda, \gamma_{\lambda c}^2)$ for this *single* system. LLM suppose the ensemble to be characterized by an $\langle M^2 \rangle$ and a $\langle D \rangle$, which are not those of the observed system because the sets $\langle M_i^2 \rangle$ and $\langle D_i \rangle$ of the observed system must exhibit sample fluctuations, shown in Table I. Therefore, the question which is the central point of the entire study of LLM is the following:

Given the $(E_\lambda, \gamma_{\lambda c}^2)$ for a single doorway, what is the probable error in taking the value of $W = 2\pi\langle M^2 \rangle / \langle D \rangle$ for the entire ensemble to be that of this doorway?

The first point to be made is that the answer to this question has little relevance to the problem of extracting useful information from, for example, the high resolution data on IAS. If this probable

error is large, the implication is simply that the spreading width is unique to a particular doorway system and that the ensemble strength function is not a useful concept. If the probable error is small, the ensemble parameter W is equal to $W_1 = 2\pi\langle M_i^2 \rangle / \langle D_i \rangle$ for the *physical* doorway system. But then the result depends on how accurately W_1 can be determined for the *physical doorway system*. Since the motivation for considering an ensemble SF was that in intermediate to weak coupling the spreading width is not meaningfully defined for the box-averaged SF favored by LLM, the purpose of the exercise is lost in either case. Thus, whatever the answer to the question, the construction of a completely fictitious ensemble with an associated SF provides no escape from the fact that the sliding-box SF is useless for a doorway state with weak coupling to neighboring fine-structure states. (Even for the case of strong coupling this SF does not have the Lorentzian form assumed by LLM.)

The second point to be made is that the answer to the question posed by LLM is the *standard deviation in the values of $W_1 = 2\pi\langle M_i^2 \rangle / \langle D_i \rangle$ for all the doorways in an ensemble, and this is determined by the distribution functions for the matrix elements and level spacings* as shown in the Appendix. The form of these ensemble *distributions* cannot be inferred from the $(E_\gamma, \gamma_{\lambda c}^2)$ of a single doorway system. Thus, the information available from a single doorway system is not sufficient to construct the ensemble.

In summary, the answer to the question posed by LLM provides no information on the root problem—how accurately can a meaningful spreading width (definition?) be determined for a single doorway system?

C. LLM results disagree with exact predictions

The study by LLM actually used the discontinuous summed SF

$$\Sigma(E) = \sum_{E_S \leq E \leq E} \gamma_{\lambda c}^2, \quad (15)$$

which was equated to

$$\int_{-\infty}^E dE' S(E') = \frac{\pi}{2} + \tan^{-1} \frac{E - E_D}{W_1/2}. \quad (16)$$

Arbitrarily chosen points on the “staircase” function $\Sigma(E)$ for each doorway system were LSQ fitted to Eq. (16) to determine a value for W_1 . This procedure was carried out for each of 100 doorway systems in four ensembles characterized by $W = \pi/2, \pi, 2\pi$, and 4π and constructed as described in this paper. A different value of W_1 was obtained for each doorway system. From these the average

$\{W_1\}$ and the standard deviation were calculated for each ensemble.

LLM found that their average $\{W_1\}$ always exceeded the ensemble parameter W by 5–8%. This difference was attributed to the effect of a finite number of levels. The fractional standard deviation of W_1 for the ensemble with $W = \pi/2$ was 44%, and the fractional standard deviations of W_1 for $W = \pi, 2\pi$, and 4π were found to be 33%, 30%, and 31%, respectively. LLM conjectured that the fractional standard deviation of W_1 would approach zero if W were increased, although this suggestion is not supported by these results. Indeed, the exact calculation of $\sigma^2(W_1)$ given by Eq. (A9) of the Appendix (which is accurately confirmed by the numerical results of this paper) shows that the fractional standard deviation σ/W is *independent of W* and equal to $[(1 + 4/\pi)/N_L]^{1/2} \approx 15\%$. The results of LLM actually confirm the *constancy* of σ/W , except for $W = \pi/2$ where a fitting procedure based on $\Sigma(E)$ should be expected to fail completely. However, their values for σ/W are too large by almost exactly a factor of 2.

VI. SUMMARY AND CONCLUSIONS

A model study on 400-fragmented doorway states has used a strength function (SF) which is the Lorentz-weighted average of reduced widths for a reactance matrix (K matrix or Wigner-Eisenbud R matrix) to study the spreading of the doorway state. The results show that this SF can be used in both weak and strong coupling to determine a spreading width $\Gamma_I^\dagger(E_D)$ that is unambiguously the Lorentz-weighted average of the squared microscopic coupling matrix elements (M_i) from the doorway to the states at (ϵ_i) . By choosing the averaging width I properly, the statistical error can easily be reduced below 10%. Moreover, for a fixed value of I the error in determining $\Gamma_I^\dagger(E_D)$ *decreases* as the coupling becomes weaker.

For each doorway system a number of average quantities were calculated— $W_1 = 2\pi\langle M_i^2 \rangle / \langle D_i \rangle$, $W_2 = 2\pi\langle M_i^2 / D_i \rangle$, $\langle \Gamma_I^\dagger \rangle$, and $[\langle (\Gamma_I^\dagger)^2 \rangle - \langle \Gamma_I^\dagger \rangle^2]$ —as well as the quantity $\Gamma_I^\dagger(E_D)$. Averages and standard deviations over an ensemble of 100 doorway systems were then calculated for each of these quantities. The ensemble averages and their standard deviations agree with exact expressions derived from the normal distribution of (M_i) and the Wigner distribution of level spacings. These averages summarize several observations which are obvious from a perusal of $\Gamma_I^\dagger(E)$ for the individual doorway systems in the ensemble:

(1) The ensemble average of $\Gamma_I^\dagger(E_D)$ is equal to $W = 2\pi\langle M^2 \rangle / \langle D \rangle^2$, but the spreading widths of about 32% of the doorway states differ from W by a

fractional amount greater than $(\pi I)^{-1/2} = \langle D \rangle / \pi I)^{1/2}$.

(2) If the doorway state is randomly placed among doorway states (ϵ_i) to which it is coupled by (preassigned) matrix elements (M_i), the probability is about 32% that the width $\Gamma_i^{\dagger}(E_D)$ will differ from the energy-averaged quantity $\langle \Gamma_i^{\dagger} \rangle$ by a fractional amount greater than $(\pi I)^{-1/2}$.

(3) The ensemble average of $W_i = 2\pi \langle M_i^2 \rangle / \langle D_i \rangle$ equals $W = 2\pi \langle M^2 \rangle / \langle D \rangle^2$, but in about 32% of the systems W_i differs from W by a fractional amount greater than 15%.

(4) The ensemble average of $W_2 = 2\pi \langle M_i^2 / D_i \rangle$ equals approximately $(\pi/2)W$.

These results establish that (1) the Lorentz-average spreading width of Feshbach, Kerman, and Lemmer¹ can be determined directly from experimental data and that (2) it is not an average parameter for a fictitious ensemble but a quantity which characterizes the spreading of the physical doorway state.

ACKNOWLEDGMENTS

The author acknowledges with pleasure the assistance of Mr. Howard Weiss, who carried out the numerical calculations described in this paper. The University of Maryland Computer Science Center provided both the computer time and the assistance of Mr. Michael Sasso to make this study possible. This research is part of the theoretical nuclear physics program supported at the University of Maryland by the Department of Energy.

APPENDIX A

All the averages and variances calculated for an ensemble of model doorway systems can be evaluated theoretically using just the distribution functions. The only quantities needed for the calculations are the averages

$$\begin{aligned} \langle 1/D \rangle &= \pi/2, \\ \langle D \rangle &= 1, \\ \langle D^2 \rangle &= 4/\pi, \\ \langle M^2 \rangle &= W/2\pi, \\ \langle M^4 \rangle &= \langle M^2 \rangle^2. \end{aligned} \quad (\text{A1})$$

Now calculate each of the following ensemble averages and the corresponding variances: (1) $\{W_1 = 2\pi \langle M_i^2 \rangle / \langle D_i \rangle\}$, (2) $\{W_2 = 2\pi \langle M_i^2 / D_i \rangle\}$, (3) $\{\Gamma_i^{\dagger}(E_D)\}$, and (4) $\{\Gamma_i^{\dagger}(E)_E\}$. Averages over the parameter for a particular doorway system are denoted by angular brackets; curly brackets denote an average over an ensemble.

Ensemble average and variance of W_1

The ensemble average of W_1 can be written

$$\{W_1\} = 2\pi \{ \langle M_i^2 \rangle \} / \{ \langle D_i \rangle \}, \quad (\text{A2})$$

since the M_i and D_i are independently drawn from different distributions. The average $\{ \langle M_i^2 \rangle \}$ is taken over (100×100) quantities, so an accurate evaluation is $\{ \langle M_i^2 \rangle \} = \langle M^2 \rangle$, giving the result

$$\{W_1\} = 2\pi \langle M^2 \rangle / \langle D \rangle = W. \quad (\text{A3})$$

The variance can be closely approximated by

$$\begin{aligned} \sigma^2(\{W_1\}) &= (2\pi)^2 \frac{\sigma^2(\{ \langle M_i^2 \rangle \})}{\{ \langle D_i \rangle \}^2} + \frac{\sigma^2(\{ \langle D_i \rangle \}) \{ \langle M_i^2 \rangle \}}{\{ \langle D_i \rangle \}^2}. \end{aligned} \quad (\text{A4})$$

To evaluate the variance

$$\sigma^2(\{ \langle M_i^2 \rangle \}) = \{ \langle M_i^2 \rangle^2 \} - \{ \langle M_i^2 \rangle \}^2 \quad (\text{A5})$$

use

$$\{ \langle M_i^2 \rangle^2 \} = \frac{1}{N_L^2} \sum_i M_i^2 M_j^2$$

with N_L the number of levels in a doorway system to get

$$\sigma^2(\{ \langle M_i^2 \rangle \}) = \sigma(\langle M^2 \rangle) / N_L. \quad (\text{A6})$$

From Eq. (A1) calculate $\sigma(\langle M^2 \rangle) = 2\langle M^2 \rangle$ to get the result

$$\sigma^2(\{ \langle M_i^2 \rangle \}) = (2/N_L) \langle M^2 \rangle. \quad (\text{A7})$$

From Eq. (A1) calculate the variance $\sigma^2(\langle D \rangle) = (4/\pi - 1)$ and use the analog of Eq. (A6) to get the variance

$$\sigma^2(\{ \langle D_i \rangle \}) = (4/\pi - 1) / N_L. \quad (\text{A8})$$

Clearly, to an excellent approximation $\{ \langle D_i \rangle \} = \langle D \rangle$ and $\{ \langle M_i^2 \rangle \} = \langle M^2 \rangle$. The variance of $\{W_1\}$ then evaluates to the result

$$\sigma^2(\{W_1\}) = W^2(1 + 4/\pi) / N_L. \quad (\text{A9})$$

Ensemble average and variance of W_2

The fact that D_i and M_i are drawn from different distributions leads to the factorization

$$\{W_2\} = 2\pi \{ \langle M_i^2 \rangle \} \times \{ \langle 1/D_i \rangle \}. \quad (\text{A10})$$

When the double averages over 10^4 levels are equated to the distribution averages in (A1), the result follows

$$\{W_2\} = W(\pi/2). \quad (\text{A11})$$

The variance of $\{W_2\}$ is

$$\begin{aligned} \sigma^2(\{W_2\}) &= (2\pi)^2 (\sigma^2(\{ \langle M_i^2 \rangle \}) \{ \langle 1/D_i \rangle \} \\ &\quad + \{ \langle M_i^2 \rangle \} \sigma^2(\{ \langle 1/D_i \rangle \})). \end{aligned} \quad (\text{A12})$$

Since $\langle 1/D^2 \rangle$ is infinite the variance of $\langle 1/D \rangle$ is infinite. The variance of $\{W_2\}$ is therefore infinite

Approximating the sum to an integral gives the result

Ensemble Average and variance of $\Gamma_I^\dagger(E_D)$

Factorization of ensemble averages of M_i and ϵ_i gives

$$\{\Gamma_I^\dagger(E_D)\} = 2I \langle M^2 \rangle \left\{ \sum_i \frac{1}{(E_D - \epsilon_i)^2 + I^2} \right\}. \quad (\text{A13})$$

$$\{\Gamma_I^\dagger(E_D)\} = \{W_1\} = W. \quad (\text{A14})$$

The variance of this ensemble average is given by

$$\sigma^2(\{\Gamma_I^\dagger(E_D)\}) = 4I^2 \left[\sigma(M^2) \sum_i \frac{1}{[(E_D - \epsilon_i)^2 + I^2]^2} + \langle M^2 \rangle \sigma(\langle D \rangle) \sum_i \frac{(E_D - \epsilon_i)^2}{[(E_D - \epsilon_i)^2 + I^2]^3} \right]. \quad (\text{A15})$$

Again, the sums can be approximately evaluated as integrals to yield the simple result

$$\sigma^2(\{\Gamma_I^\dagger(E_D)\}) = W^2 \left(\frac{1}{\pi I} \right) \left(1 + \frac{4/\pi - 1}{2I^2} \right). \quad (\text{A16})$$

Ensemble average and variance of $\langle \Gamma_I^\dagger(E) \rangle$

The quantity $\langle \Gamma_I^\dagger(E) \rangle$ is an energy average of $\Gamma_I^\dagger(E)$. In the model this quantity was calculated by averaging over the integral $175 < E \leq 225$. The interval will be taken as $E_D - \Delta/2 < E < E_D + \Delta/2$ in evaluating the ensemble average $\{\langle \Gamma_I^\dagger(E) \rangle\}$, but the result is evaluated in the limit of Δ very large. The ensemble average is then

$$\{\langle \Gamma_I^\dagger(E) \rangle\} = \frac{1}{\Delta} \int_{E_D - \Delta/2}^{E_D + \Delta/2} dE 2I \sum_i \frac{\{M_i^2\}}{\{(E - \epsilon_i)^2 + I^2\}}. \quad (\text{A17})$$

Approximate evaluation of this expression gives

$$\{\langle \Gamma_I^\dagger(E) \rangle\} = \{W_1\} = W. \quad (\text{A18})$$

The variance of the ensemble average of $\langle \Gamma_I^\dagger \rangle$ is approximately equal to the variance of W ,

$$\{\langle \Gamma_I^\dagger \rangle^2\} - \{\langle \Gamma_I^\dagger \rangle\}^2 = W^2(1 + 4/\pi)/N_L. \quad (\text{A19})$$

Still another variance can be calculated for $\langle \Gamma_I^\dagger \rangle$, viz., $\langle (\Gamma_I^\dagger)^2 \rangle - \langle \Gamma_I^\dagger \rangle^2$. Naturally this quantity also depends very much on the particular doorway system, so let us average over the ensemble. First evaluate the average of $(\Gamma_I^\dagger)^2$.

$$\langle (\Gamma_I^\dagger)^2 \rangle = \frac{4I}{\Delta} \sum_i \left[\frac{M_i^2 M_i^2}{(\epsilon_i - \epsilon_j)^2 + 4I^2} \tan^{-1} \frac{E - \epsilon_i}{I} + \tan^{-1} \frac{E - \epsilon_i}{I} - \frac{I}{\epsilon_i - \epsilon_j} \ln \frac{(E - \epsilon_i)^2 + I^2}{(E - \epsilon_j)^2 + I^2} \right]_{E_D - \Delta/2}^{E_D + \Delta/2}. \quad (\text{A20})$$

When this expression is evaluated at the limits for large Δ , the second term is found to be negligible compared to the first term. In evaluation of the ensemble average of the first term, it is necessary to distinguish between the terms for $i=j$ and those for which $i \neq j$. The result is

$$\{\langle (\Gamma_I^\dagger)^2 \rangle\} = W^2 \left(1 + \frac{1}{\pi I} \right). \quad (\text{A21})$$

The ensemble average $\{\langle \Gamma_I^\dagger \rangle^2\}$ evaluates in the limit of large Δ to W^2 . This leads to the ensemble average

$$\{\langle (\Gamma_I^\dagger)^2 \rangle\} - \{\langle \Gamma_I^\dagger \rangle^2\} = W^2/\pi I. \quad (\text{A22})$$

In the text, the ensemble averages given in Eqs. (A3), (A10), (A11), (A14), (A16), (A18), (A19), and (A22) are compared with those calculated directly from a model ensemble with $W = 2\pi$. The results are presented in Tables I, II, III, and IV.

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