Neutron Resonance Widths and the Porter-Thomas Distribution

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Experimental evidence has recently put the validity of the Porter-Thomas distribution (PTD) for partial neutron widths into question. We identify two terms in the effective Hamiltonian that violate orthogonal invariance (the basis for the PTD). Both are due to the coupling to the decay channels. We show that realistic estimates for the coupling to the neutron channel and for nonstatistical γ decays yield significant modifications of the PTD, similar to the observed ones.

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Introduction.—Recent experimental results on the distribution of neutron resonance widths have cast serious doubt on the validity of random-matrix theory (RMT) in nuclei. RMT predicts that the reduced neutron widths follow a Porter-Thomas distribution (PTD) [1] (a χ^2 distribution with a single degree of freedom, $\nu = 1$). That prediction assumes nonoverlapping resonances with a single open channel (the neutron channel). A maximum-likelihood analysis of neutron widths in two Pt isotopes using a χ^2 distribution with ν degrees of freedom gave $\nu = 0.47$ and $\nu = 0.57$, excluding the PTD with high statistical significance [2]. For the Nuclear Data Ensemble, the analysis resulted in ν values significantly larger than unity [3,4]. Numerous theoretical attempts [5–9] to account for the results of Refs. [2,3] have not definitively resolved the issue. The validity of RMT is of central importance for the statistical theory of nuclear reactions [10] that is widely used in nuclear cross section calculations.

In the present Letter we address two dynamical effects that modify the PTD and that apparently have not been taken into account so far in the theoretical literature or in the analysis of neutron resonance data. The two effects are the Thomas-Ehrman shift known from the study of light nuclei [11], and nonstatistical effects in the γ decay of the neutron resonances [12]. We show that both may cause significant deviations of the distribution of neutron resonance widths from the PTD.

The PTD follows from the orthogonal invariance of the Gaussian orthogonal ensemble of random matrices (the GOE). The GOE distribution function is proportional to

$$d\mathcal{O}\exp\left\{-\frac{N}{\lambda^2}\sum_\rho E_\rho^2\right\}\prod_{\mu<\nu}^{N}|E_\mu - E_\nu|\prod_\sigma^N dE_\sigma. \quad (1)$$

Here N with $N \to \infty$ is the dimension of the GOE matrices. The parameter λ defines the width 4λ of the GOE spectrum. The mean level spacing at the center of the GOE spectrum is $d = \pi\lambda/N$. The E_μ are the GOE eigenvalues, and $d\mathcal{O}$ is the Haar measure of the orthogonal group in N dimensions. It encompasses the GOE eigenfunctions. Factorization of the distribution implies that eigenvalues and eigenfunctions are statistically independent. For $N \to \infty$, the projections of the eigenfunctions onto an arbitrary vector in Hilbert space possess a Gaussian distribution, and the reduced widths, therefore, have a PTD. The reported disagreement of the distribution of reduced neutron widths with the PTD directly challenges the postulated orthogonal invariance of the GOE. Conversely, dynamical effects that violate orthogonal invariance will cause deviations from the PTD. We show that both, the Thomas-Ehrman shift and nonstatistical γ decays, have that property and, thus, qualify as causes of the observed disagreement.

Violation of orthogonal invariance.—We consider s-wave neutron scattering on a spin zero target nucleus. We take account of the single open neutron channel and of the large number of γ decay channels. The effective Hamiltonian is [10]

$$H_{\mu\nu}^{\rm eff} = H_{\mu\nu}^{\rm GOE} + F_{\mu\nu}(E) - i\pi W_\mu(E)W_\nu(E) - i\pi\sum_\gamma W_\mu^{(\gamma)}W_\nu^{(\gamma)}. \quad (2)$$

Here E is the neutron energy. We have replaced the actual Hamiltonian by the GOE Hamiltonian $H^{\rm GOE}$ as defined in Eq. (1). The real matrix elements $W_\mu(E)$ with $\mu = 1, 2, \ldots, N$ couple the s-wave neutron channel to the space of N resonance states and carry the same energy dependence $E^{1/4}$ as do the neutron partial width amplitudes. The shift matrix F accounts for that energy dependence. It is the analog of the Thomas-Ehrman shift, with elements

$$F_{\mu\nu}(E) = {\rm P}\int_0^\infty dE'\frac{W_\mu(E')W_\nu(E')}{E - E'} \quad (3)$$

where P indicates the principal-value integral. At energies far above the threshold, the matrix F is often neglected because then contributions to the integral from energies $E' < E$ and $E' > E$ tend to cancel. Such cancellation cannot occur at the neutron threshold $E = 0$ and $F_{\mu\nu}(E)$ may, thus, not be negligible. We neglect contributions similar to F from closed channels and take $F(E)$ as a paradigmatic example. The matrix elements $W_\mu^{(\gamma)}$ play the same role for the γ channels as do the W_μ for the neutron channel except for a different energy dependence of the $W_\mu^{(\gamma)}$, resulting in a negligible contribution to the Thomas-Ehrman shift.

None of the terms added to $H^{\rm GOE}$ in Eq. (2) is invariant under orthogonal transformations. Addressing the regime of isolated resonances we confine our attention to the matrix F and to the coupling to the γ decay channels. Thus, the elements of the width matrix $W_\mu W_\nu$ only serve to define the neutron decay widths and are otherwise negligible. Beyond that regime, the width matrix does cause deviations from the PTD [6,7].

Let us first disregard γ decay channels and concentrate on the role of F. Writing $W_\mu(E) = \mathcal{W}_\mu E^{1/4}$ we observe that the matrix $\mathcal{W}_\mu \mathcal{W}_\nu$ has a single nonzero eigenvalue $\sum_\mu \mathcal{W}_\mu^2$. The associated eigenvector defines the superradiant state [13,14] labeled $\mu = 1$. The transformation to the eigenvector basis leaves the ensemble of GOE matrices unchanged and yields

$$H^{\rm eff}_{\mu\nu} \approx H^{\rm GOE}_{\mu\nu} + \delta_{\mu 1}\delta_{\nu 1}\left[F - i\pi\sum_\rho W_\rho^2(E)\right] \qquad (4)$$

where $F = \sum_\mu F_{\mu\mu}$.

The transformation does not diagonalize the matrix F exactly because the integral defining F receives contributions also from higher energies where the approximation $W_\mu(E) \approx \mathcal{W}_\mu E^{1/4}$ does not apply. Near the neutron threshold such contributions are relatively small, however, and Eq. (4) should be a good approximation.

We compare F [Eq. (4)] with the diagonal element $H^{\rm GOE}_{11}$. Sufficiently far above the neutron threshold (where the s-wave penetration factor is ≈ 1) the matrix elements W_μ obey [10] $\sum_\mu W_\mu^2 = N dx/\pi^2$ where x is related to the average of the s-wave scattering function via $\bar{S} = (1-x)/(1+x)$ and is, thus, of order unity. Hence, $\sum_\mu W_\mu^2 \approx dN/\pi^2 = \lambda/\pi$. For $N \gg 1$ that is much larger than the root-mean-square value $\lambda\sqrt{2/N}$ of the diagonal element $H^{\rm GOE}_{11}$. For $E \to 0$ the s-wave penetration factor reduces $\sum_\mu W_\mu^2$. The reduction does not affect the principal-value integral, however, which actually attains its maximum value at $E = 0$. Thus, we expect $F \approx \lambda/\pi$. The effect of F can be amplified beyond our estimate by a single-particle resonance near the neutron threshold. Such is the case in the Pt isotopes for the 4s state of the shell model [5].

Next, we turn to the γ channels in Eq. (2). According to the statistical model, the matrix elements $W_\mu^{(\gamma)}$ are Gaussian-distributed random variables. The total γ widths of the neutron resonances are, therefore, expected to have a χ^2 distribution with a large number of degrees of freedom, and the partial widths $\Gamma_\mu^{(\gamma)}$ of the neutron resonances in a given target nucleus are expected to have nearly the same value. The effective Hamiltonian is, thus, expected to be approximately given by $H^{\rm eff}_{\mu\nu} = H^{\rm GOE}_{\mu\nu} - i\pi W_\mu W_\nu - \delta_{\mu\nu} i\bar{\Gamma}/2$, with $\bar{\Gamma}$ independent of μ. The term $\delta_{\mu\nu} i\bar{\Gamma}/2$ is obviously orthogonally invariant. While the contribution of each γ channel to $\bar{\Gamma}$ is small, the number of such channels is large resulting in a value of $\bar{\Gamma}$ that dominates the total neutron resonance widths near the neutron threshold.

A recent analysis [12] of the distribution of total γ decay widths of neutron resonances in ^{96}Mo contradicts the expectation that these all have the same value. For s-wave resonances and positive parity states, the distribution is shown in the lower part of Fig. 6 of Ref. [12]. The distribution is much wider than predicted by the GOE. The result confirms earlier data [15] comprising a much smaller number of resonances. It seems that at present, the cause for the deviation is not understood. It is not clear whether it is due to a specific property of ^{96}Mo or whether it is likely to occur in other nuclei as well. We opt for the second possibility. We assume that the total γ decay widths generically possess large fluctuations, in contradiction to the statistical model. We explore the consequences of that hypothesis for the distribution of neutron decay widths.

Typical values of total γ decay widths for s-wave neutron resonances are of order 100 meV, both in medium-weight [12] and in heavy [16] nuclei. The distributions for the total γ decay widths shown in Ref. [12] start roughly at $\Gamma_0 = 100$ meV and fall off with a half width σ of roughly 300 meV. To transcribe these figures into the effective Hamiltonian of Eq. (2) we use that in medium-weight and heavy nuclei typical average resonance spacings $d = \pi\lambda/N$ are of order 10 eV. Then $\Gamma_0 \approx \pi\lambda/(100N)$ and $\sigma \approx \pi\lambda/(30N)$. The orthogonal invariance of the coupling to the γ decay channels is broken by the spread σ. We compare σ with the Thomas-Ehrman shift function $F \approx \lambda/\pi$. We have $(1/N){\rm Tr}\sigma \approx \pi\lambda/(30N)$ while $(1/N){\rm Tr}(F\delta_{\mu 1}\delta_{\nu 1}) = F/N = \lambda/(\pi N)$. While somewhat smaller, γ decay breaks orthogonal invariance roughly as strongly as does the Thomas-Ehrman shift.

In summary we have identified two effects that break the orthogonal invariance of the GOE, the Thomas-Ehrman shift and the nonstatistical distribution of γ decay widths. In the remainder of the Letter we investigate the consequences of both effects for the distribution of neutron resonance widths. We do so in the framework of a schematic model. We write the effective Hamiltonian as

$$H^{\rm eff} = H^{\rm GOE}_{\mu\nu} + \delta_{\mu 1}\delta_{\nu 1} Z. \qquad (5)$$

We have suppressed the constant γ decay width $\bar{\Gamma}$ because it only causes a uniform shift of all eigenvalues [8] and does not affect the eigenfunctions. The constant

$$Z = F - (i/2)\delta\Gamma - i\pi\sum_{\rho} W_{\rho}^2 \qquad (6)$$

violates orthogonal invariance and includes the Thomas-Ehrman shift; the effect of nonstatistical γ decays where we schematically represent the spread of γ decay widths by a single term; and the term $-i\pi\sum_{\rho} W_{\rho}^2$ which is a reminder that we use a basis where the state $|1\rangle$ is the superradiant state.

Average level density.—It is easy to see that for $N \to \infty$ the presence of Z in the effective Hamiltonian has a negligible influence on the average level density. The level density is defined as $\rho(E) = -(1/\pi)\Im(E^+ - H^{\mathrm{eff}})^{-1}$. Here $(E^+ - H^{\mathrm{eff}})^{-1}$ is the retarded Green function. This expression for ρ is physically meaningful only if H^{eff} is Hermitian, i.e., if Z is real. We first consider that case and put $Z = F$. The term F in H^{eff} may be considered as corresponding to a doorway state. Therefore, we treat the first line and the first column of H^{eff} differently from the rest [14]. We define the orthogonal projection operators $P = |1\rangle\langle 1|$ and $Q = 1 - P$. With $\mu, \nu \geq 2$ we write $PH^{\mathrm{eff}}P = H_{11}^{\mathrm{GOE}} + Z = E_0$, $(PH^{\mathrm{eff}}Q)_{1\mu} = H_{1\mu}^{\mathrm{GOE}} = V_{\mu}$, $(QH^{\mathrm{eff}}Q)_{\nu 1} = H_{\nu 1}^{\mathrm{GOE}} = V_{\nu}$, and $(QH^{\mathrm{eff}}Q)_{\nu\mu}$. The elements of the matrix $QH^{\mathrm{eff}}Q$ are Gaussian-distributed random variables. Moreover, the probability distribution of $QH^{\mathrm{eff}}Q$ is invariant under orthogonal transformations in Q space. Therefore, the matrices $QH^{\mathrm{eff}}Q$ form a GOE of dimension $N - 1$. We denote that ensemble by $\tilde{H}^{\mathrm{GOE}}$ and, suppressing the term $\sum_{\rho} W_{\rho}^2$, write the total Hamiltonian in matrix form,

$$H^{\mathrm{eff}} = \begin{pmatrix} E_0 & V_{\mu} \\ V_{\nu} & \tilde{H}_{\nu\mu}^{\mathrm{GOE}} \end{pmatrix}. \qquad (7)$$

The right-hand side of Eq. (7) is identical in form with the standard model for a doorway state (see, for instance, Ref. [17]). The spreading width of the doorway state is $\Gamma^{\downarrow} = 2\pi(1/N)\sum_{\mu} V_{\mu}^2/d$. In the present case we have $\sum_{\mu} V_{\mu}^2 = \sum_{\mu} H_{1\mu}^2$. We note that for $N \gg 1$ the sum is self-averaging and given by λ^2 for every member of the ensemble (7). The resulting value of the spreading width $\Gamma^{\downarrow} = 2\lambda$ is comparable with the total width of the GOE spectrum, and the doorway state is completely smeared over that spectrum. While in the standard doorway-state model [17], the magnitude of the coupling matrix elements V_{μ} is of order d, here their root-mean square values $d\sqrt{N}$ are fixed by the underlying GOE and very large compared to d. Therefore, the doorway state does not cause a local enhancement of the level density. We note that the model of Eq. (7) is physically meaningful only for $|Z| \leq 2\lambda$. For $|Z| \gg 2\lambda$ there exists a distinct state outside the GOE spectrum that carries (almost) all the coupling to the neutron channel. That case does not seem to model the scattering of slow neutrons in a meaningful way.

As a corollary we mention that for imaginary Z and $|Z| \approx 2\lambda$ we deal with a superradiant state that causes a pole of the Green function in the complex energy plane. The distance of that pole from the real axis is comparable with the width of the GOE spectrum. Therefore, the superradiant state conveys only a small part of its large neutron width to the remaining GOE eigenstates. It does not seem meaningful to consider imaginary values of Z in excess of 2λ.

Numerical results.—With ϕ_{μ} the normalized eigenfunctions of the effective Hamiltonian [Eq. (5)] with $\sum_{\rho} W_{\rho}^2 \to 0$, the partial neutron decay widths are proportional to $N|\langle 1|\phi_{\mu}\rangle|^2$. The factor N is introduced so that the average width equals unity. We have calculated the effect of Z on the distribution of partial widths $x = N|\langle 1|\phi_{\mu}\rangle|^2$ perturbatively, both for $|Z| \ll d$ and for $|Z| \gg \lambda$. The results show that Z does influence the PTD. Both limits are unrealistic, however, and serve only as a check for the numerical work. Therefore, we do not give our analytical results here.

We first present results for real Z. We use the dimensionless parameter $\kappa = Z/\lambda$ and consider values that are physically realistic but lie outside the range of validity of the perturbative approach. As Z increases the PTD $P(x) = [1/(2\sqrt{2\pi x})] \exp\{-x/2\}$ is deformed. The resulting probability distribution $\mathcal{P}(x)$ of the partial widths is shown in a plot of $[\mathcal{P}(x)/P(x)] - 1$ versus x for several values of κ in Fig. 1. The term $Z|1\rangle\langle 1|$ in H^{eff} leads to a segregation of states. The states in one group become broader and those in the other group become more narrow. Therefore, the modified distribution has a longer tail and is more strongly peaked at $x = 0$ than the PTD, while in the middle around $x = 1$ the distribution is suppressed. In the limit of very large κ one state becomes collective (i.e., carries almost all the decay strength). The distribution of widths of the remaining states returns to the PTD but with a much reduced average width. That is consistent with our perturbative results for large Z.

We have fitted these curves using the parametrization

$$\mathcal{P}(x) = [1 + A(1 - x) + B(x^2 - 6x + 3)]P(x) \qquad (8)$$

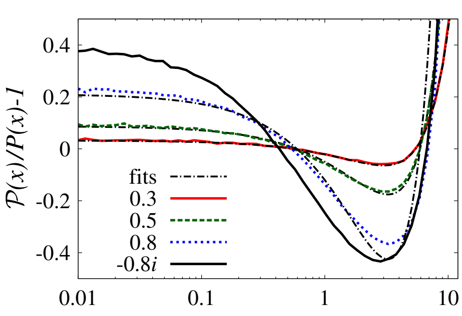

FIG. 1 (color online). Relative difference $[\mathcal{P}(x)/P(x)] - 1$ as a function of x for several values of κ as indicated in the figure and for $N = 1000$. The dashed-dotted lines are fits using expression (8).

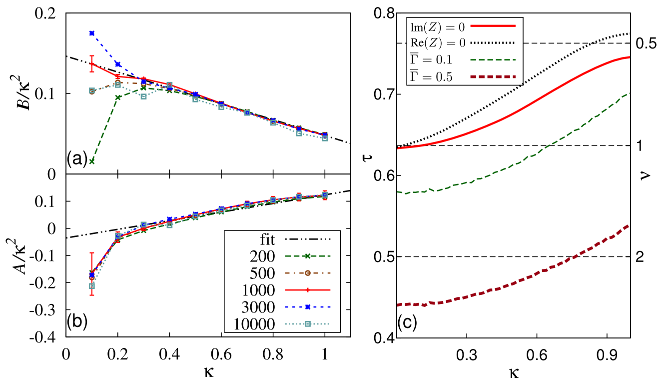

FIG. 2 (color online). Scaled fit coefficients: (a) B/κ^2 and (b) A/κ^2 with A and B defined in Eq. (8) are plotted as functions of κ for GOE ensembles of different dimensions N as indicated in the figure. For $N = 1000$ the error in the fit is shown by error bars. The errors for the other curves are similar. The double-dot-dashed black line shows the linear fits [Eq. (9)] of A/κ^2 and B/κ^2 as functions of κ. Right: (c) The coefficient τ defined in Eq. (10) is plotted versus κ for different widths of multiple random γ channels as explained in the text. The scale on the right shows the corresponding ν values.

suggested by the perturbative result for small Z. The distribution $\mathcal{P}(x)$ in Eq. (8) is normalized to unity for all values of A and B. Terms linear (quadratic) in x embody a change in average width (a quenching of the PTD, respectively). For each of the curves representing the data we also show a fit using Eq. (8) as a dashed-dotted line. In the interval $0.1 \le \kappa \le 1$ that is most relevant for applications, the deviations from the PTD are described perfectly by Eq. (8).

The scaled fit coefficients A/κ^2 and B/κ^2 are shown as functions of κ in Fig. 2 for different matrix dimensions N. For $\kappa < 0.4$ we encounter numerical instabilities. However, in that regime the changes of the PTD are too small to be of practical interest. For $\kappa > 0.4$ the results for different matrix dimension N exhibit consistently a linear dependence on κ approximately given by

$$A/\kappa^2 = -0.035 \pm 0.010 + (0.16 \pm 0.01)\kappa,$$
$$B/\kappa^2 = 0.146 \pm 0.002 - (0.099 \pm 0.003)\kappa. \qquad (9)$$

As a single quantitative measure of deviations from the PTD we use the coefficient of the L variation (also known as the Gini coefficient) defined as

$$\tau = \frac{1}{2\bar{x}} \int dx \int dx' |x - x'| \mathcal{P}(x) \mathcal{P}(x'). \qquad (10)$$

The advantage of using τ over the traditional coefficient of variation is that τ is nearly insensitive to the existence of a small fraction of highly collective states that may compromise the average value of x [7]. The coefficient τ ranges between zero and unity. For a χ^2 distribution with $\nu = 1$ and $\nu = 2$ we have $\tau = 2/\pi$ and $\tau = 1/2$, respectively; τ decreases with increasing ν. A value of $\tau > 2/\pi \approx 0.64$ corresponds to a distribution that is more strongly peaked at small x than the PTD and effectively has $\nu < 1$. For a distribution of the form, Eq. (9), we find $\tau = (2/\pi)(1 - 2A - A^2 + 2B - 2AB - 3B^2)$. The results for purely imaginary Z are qualitatively similar to those for real Z. Compared to the PTD, the distribution is increased for small and large x and is depressed for $x \approx 1$. That is shown for $Z/\lambda = -0.8i$ by the black solid line in Fig. 1. For imaginary Z we do not present a fit because we have not succeeded in finding similarly good fit formulas as in Eqs. (9) for real Z. Results for real and for complex values of Z are shown in Fig. 2(c) where τ is plotted as a function of κ. The case $\mathrm{Im}(Z) = 0$ corresponds to Eqs. (9). When $\mathrm{Re}(Z) = 0$ we define $\kappa = |Z|/\lambda$. The figure also includes curves where the Thomas-Ehrman shift [Eq. (5)] is combined with the effect of multiple γ channels. For the latter, in addition to the schematic model Eq. (6) for the neutron channel, we have assumed that the γ decay widths have a random distribution with mean value $\bar{\Gamma}$ (in units of the average neutron width) and a variance as estimated above.

Conclusions.—The PTD follows from the orthogonal invariance of the GOE. We have identified two causes for violation of that invariance: the Thomas-Ehrman shift and nonstatistical γ decays. Invariance breaking by the Thomas-Ehrman shift is due to the coupling to the neutron channel. Such coupling is immanent in the theory and does not invalidate the GOE. In contradistinction, it may be argued that the existence of nonstatistical γ decays represents a genuine violation of GOE assumptions. It is conceivable that such decays are due to transitions to low-lying states where random-matrix theory does not apply.

We have shown that reasonable estimates of both violations yield significant deviations of the distribution of neutron decay widths from the PTD. The deviations cover the range of ν values found in Refs. [2,3]. The Thomas-Ehrman shift is strongest at the neutron threshold and is expected to be particularly pronounced when the s-wave strength function is maximal as is the case for the Pt isotopes. For the nuclear data ensemble the effects of nonstatistical γ decays have to be reevaluated.

In all cases studied, invariance breaking results in a depletion of the probability distribution for the partial widths x near $x = 1$, compensated by an increase for small and large values of x. To estimate the effect of such breaking in an individual nucleus, the quantities F and $\delta\Gamma$ in Eq. (6) must be estimated. For F that should be possible using the neutron strength function. For $\delta\Gamma$ (a measure of the spread of total γ decay widths) the simultaneous analysis of the distribution of partial neutron widths and of total γ decay widths for the measured neutron resonances is required.

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