

Symmetries and Quantum Chaos: Time-Reversal Invariance in the Nucleon-Nucleon Interaction

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Let α be the relative norm of a symmetry-breaking term in the Hamiltonian of a many-particle system, and Λ the energy-dependent transition parameter which characterizes the quantum chaos via spectral and strength fluctuations. Combining a compact theory for Λ/α^2 with fluctuation theories by which Λ can be deduced from (neutron-resonance) data gives, for the time-reversal-noninvariant nucleon-nucleon interaction, $\alpha \leq (1-2) \times 10^{-3}$, which would improve with better small-strength data in nuclei with dense spectra. Diffusion equations involving Λ as the "time" variable are also discussed.

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Our principal purpose is to understand the way in which the nature of quantum chaos, as characterized by spectral (energy level) and strength fluctuations, varies when a good symmetry is gradually broken, i.e., as $H = h(1) + V(k) \rightarrow H_a = H + \alpha U(p)$, where $V(k)$ is a k -body operator; we shall often have $k = p = 2$ and will then define the symmetry-breaking operator U to have, in the two-particle space, the same norm as the symmetry-preserving V . The choice of U to be representable by an imaginary antisymmetric matrix will accommodate our first application, that of determining from observed nuclear quantum chaos values for or bounds upon $\alpha \geq 0$, the relative time-reversal-nonvariant (TRNI) component of the nucleon-nucleon interaction.¹ The problem breaks into two parts.² The $\alpha \leftrightarrow \Lambda$ part is to calculate, from H_a , the energy-dependent transition parameter $\Lambda = \alpha^2 |U_{ij}|^2 / D^2$, the mean squared admixing matrix element between neighboring states measured in units of the local spacing D ; our solution of this problem will apply, or extend immediately, to symmetries other than time-reversal invariance (TRI) and to the more general problem of calculating excitation strengths in complicated systems. The "A problem" is that of deducing, from the data, values or bounds for Λ . This is simple when, as, e.g., with parity, the symmetry breaking is detected by the occurrence of an otherwise forbidden process, but is complicated when, as with TRI, Λ derives from fluctuations² or via detailed-balance experiments.³ Though the mere existence of a nonzero Λ could be of interest, indicating the occurrence of a symmetry breaking, the significance, *if any*, of an upper bound on Λ will usually not be obvious, so that the further $\Lambda \rightarrow \alpha$ analysis is essential.

From its definition we recognize that Λ/α^2 is the locally smoothed (sm) value, for $x \approx y$ in the energy region of interest, of the bivariate strength density $S(y, x)$, defined with U as the excitation operator; thus, with m the number of "active" particles (those in single-particle states neither essentially filled nor empty), Γ the conserved quantum numbers ($= J, J_z, T, T_z, \pi$ when one deals with nuclear TRI, as we shall mostly take for granted in what

follows),

$$\begin{aligned} S^{h,m,\Gamma}(y,x) &= I^{h,m,\Gamma}(y) | \langle y | U | x \rangle |^2 I^{h,m,\Gamma}(x) \\ &= \langle \langle U^\dagger \delta(H-y) U \delta(H-x) \rangle \rangle^{m,\Gamma} \\ &\rightarrow \Lambda / \alpha^2. \end{aligned} \quad (1)$$

Here $\langle \langle \rangle \rangle$ indicates the trace, $|x\rangle$ and $|y\rangle$ the H eigenstates, and $I^{h,m,\Gamma}(x) = \langle \langle \delta(H-x) \rangle \rangle^{m,\Gamma}$ gives, when smoothed, the level density $[D^{m,\Gamma}(x)]^{-1}$. It is good to start with noninteracting particles (NIP), $H \rightarrow h$; then, in h -diagonal representation, when $m \gg p$ the matrix elements of $U(p)$ necessarily lie in a narrow diagonal band [since $U(p)$ simultaneously transfers only a fraction $\leq p/m$ of the particles]. This implies that the x, y variables in the bivariate density $S^{h,m,\Gamma}$ are strongly correlated, the density peaking along the line $x \approx y$. Since the h eigenstates are m -fold products of single-particle eigenstates it is not difficult, even when good symmetries are specified, to give the *exact* strength density, in terms of eigenvalue densities, for an arbitrary excitation operator. But it will be adequate for us to deal with large spaces for which we can disregard those matrix elements of U , e.g., U_{ijk} , which transfer fewer than p particles. Ignoring Γ to begin with, we find a propagation equation for the m -particle strength density in the form of a bivariate convolution,

$$\begin{aligned} S^{h,m} &= T^{h,m-p} \otimes S^{h,p}, \\ T^{h,m}(u,v) &= \delta(u-v) I^{h,m}(u). \end{aligned} \quad (2)$$

To appreciate the nature of this result take, for example, U to have p -particle matrix elements essentially equal in magnitude, the single-particle spectrum to be finite and nonsingular, and m large enough so that, by the central limit theorem,⁴ $I^{h,m}$ is Gaussian. Then using additivity of bivariate cumulants under convolution, we find $S^{h,m}$ to be close to an "almost singular" bivariate Gaussian, almost singular because the x, y correlation coefficient is $\zeta_h = 1 - p/m$ so that the distribution for large m becomes extremely sharp in the variable $x - y$, as predicted above.

The strong positive correlation between the variables x, y survives when V is turned on because V admixes and spreads the h eigenstates over a narrow energy range, typically ± 2 MeV for heavy nuclei in the resonance region. This gives an enhancement of the admixing matrix element and an increase in the sensitivity of deducing α from Λ . A separate enhancement in sensitivity² arises from the $d^{-1/2}$ compression of the level spacing D due to the effect of distant levels (d here being the "effective" dimensionality, roughly the number of interacting states in the spreading interval above). Without these enhancements no interesting α bound would emerge from TRI fluctuation studies.

It is known that the spreading is Gaussian and more-over⁵ that the spreading width is closely constant for excitation energies of interest to us (at higher energies it increases slowly with energy). The initial and final state densities have therefore the form $I^{H,m} = I^{h,m} \otimes \rho_G^{(1)}$ where $\rho_G^{(1)}$ is (univariate) Gaussian with unit integral, zero centroid, and m -particle variance $\sigma^2(m)$, related⁴ to the defining k -particle variance by $\sigma^2(m) = \binom{m}{k} \sigma^2(k)$. For a heuristic derivation of S we assume now that the strength "follows" the densities so that the interacting-particle strength density becomes a convolution of the NIP density with a (unit integral) bivariate Gaussian spreading function $\rho_G^{(2)}$; thus

$$S^{H,m} = S^{h,m} \otimes \rho_G^{(2)} \\ = \{ \langle \langle U^\dagger U \rangle \rangle^m \}^{-1} S^{h,p} \otimes T^{h,m-p} \otimes S^{V,m}, \quad (3)$$

where the final form comes by consideration of $h=0$. With $h \rightarrow V$ in (1) we have, as the exact moments of $S^{V,m}$, $M_{rs} = \langle \langle V^r U^\dagger V^s U \rangle \rangle^m$ which, with $r+s \leq 2$, determines the six Gaussian parameters. (Note incidentally that for small spaces $S^{H,m}$ will itself be a bivariate Gaussian.⁶) Since for TRI we have no form for U it is natural to regard it as a random operator, specifically, one defined in the p -particle space by an imaginary antisymmetric random matrix, and to perform then the ensemble average. Thus, using (1), we have

$$S^{h,p}(u,v) = d^{-2}(p) \langle \langle U^\dagger U \rangle \rangle^p I^{h,p}(u) I^{h,p}(v).$$

Moreover, for $r=0$ or $s=0$ the moment traces factor and the marginal densities of $S^{V,m}$ coincide with $d(m)^{-1} \langle \langle U^\dagger U \rangle \rangle^m I^{V,m}$ in line with the heuristic argument. For the correlation coefficient ζ_V we need⁴

$$\langle \langle U^\dagger V U V \rangle \rangle^m \rightarrow \langle \langle U^\dagger U \rangle \rangle^m \sigma^2(m-p),$$

and then

$$\zeta_V \rightarrow \sigma^2(m-p) / \sigma^2(m) \sim 0.80 \pm 0.05$$

for the spaces considered below. The intuitive argument involved here is that, since U_{ij} must couple with U_{ij}^\dagger , the number of particles "available" for the operation of V is reduced by p ; a formal derivation gives also a Pauli-blocking correction. We mention too that a derivation of

(3) follows by our taking V to be a k -body embedded⁴ Gaussian orthogonal ensemble (GOE) (i.e., defined in the k -particle space but operating in an $m > k$ -particle space) and then evaluating the low-order moments for large m ; shell-model and partitioning tests have shown that this ensemble is adequate for our spaces. The variances need to evaluate $S^{H,m}$ follow directly⁵ from the matrix elements of V , and the NIP eigenvalue densities by spectral averaging involving low-order partitioned h moments.⁷

The parity and T_z quantum numbers, dropped above, are restored by a simple partitioning. For the angular momentum the same J decomposition via a spin-cutoff factor which is encountered in the theory of level densities is appropriate also for the strength density; the cutoff factor itself is easily calculable. The spreading widths and the correlation coefficient ζ_V are essentially J independent, this arising from the fact that the correlation coefficient between V and J_z^2 (whose expectation value gives the spin-cutoff factor) is small, typically ≤ 0.03 . For heavy nuclei, which give the best fluctuation bounds for TRI, isospin (T) is irrelevant.

The calculations are simple, once the model space, the single-particle energies, and the interaction V have been decided upon and tested. For heavy nuclei the first two come by inspection of the zero-deformation Nilsson spectrum which, e.g., makes plausible that for ²³²Th eight active protons should be distributed over $h_{9/2}$, $i_{13.2}$, and $f_{7/2}$, and 17 neutrons over $g_{9/2}$, $k_{15/2}$, $i_{11/2}$, and $d_{5/2}$, the gross dimensionality being $\binom{32}{8} \binom{44}{17} \sim 7 \times 10^{18}$. We choose for V a surface-delta interaction, perhaps the one best studied for heavy nuclei, and verify that the calculated level density fits experiment for a reasonable interaction strength G (which turns out to be 0.17 MeV for ¹⁶⁷Er and 0.13 MeV for ²³³Th), and is stable under small extensions of the model space. In the slow-neutron resonance region, with $J = \frac{1}{2}^+$, we find, using an early version of (3), that $\Lambda/a^2 = 3900, 730, 11600$, and 6000 , respectively, for ^{167,169}Er, ²³³Th, ²³⁹U, and, with $J = 3^-$, $\Lambda/a^2 = 1.08 \times 10^5$ for ²³⁶U, these being the nuclei needed below the TRI. The spacings for these nuclei are 38, 100, 17, 21, and 1.1 eV so that, at the resonance energies, $\Lambda D/a^2$ is essentially constant, this implying that, other things being equal, the best α bounds will come from dense spectra (small D) found in heavy nuclei. Moreover, since D decreases with angular momentum J , odd-target ($J_t \neq 0$) nuclei, which give $J = J_t \pm \frac{1}{2}$ resonances, will do better than even targets ($J_t = 0$) if the two J values can be separated, as in a polarized experiment.

We turn now to the Λ problem for the TRI, the theory for which derives from the ensemble² $\{H_a\}$ which interpolates between the Gaussian orthogonal ($\alpha=0$) and unitary ($\alpha=1$) ensembles. Once the transition theory is known, values for or bounds on Λ can be determined directly from experimental data. This is so because the

theory applies not only to ensembles but equally well to the individual realistic systems described above. For the spectral Λ problem see Ref. 2. For the strengths the main TRNI effect is that the locally renormalized strength density makes a transition from a χ_1^2 (Porter-Thomas) form to χ_2^2 . Let $|\lambda\rangle$ be the renormalized projection of the final state of the excitation into the d -dimensional statistical space in which $\{H_a\}$ operates.⁸ For each member of the fixed- α ensemble we consider the strength to the j th H_a eigenstate, the ordering being by energy. For a simple notation we write the corresponding energy E_{aj} , a mildly fluctuating random variable (variance $\sim \pi^{-2}D^2 \ln d$), as E , and the complex eigenvector as $|E\rangle = t|R\rangle + i(1-t^2)^{1/2}|I\rangle$ with the phase chosen so that the real and imaginary parts of $|E\rangle$ are orthogonal, $\langle R|I\rangle = 0$. Renormalized to unit mean, the strength, the absolute square of the overlap between $|\lambda\rangle$ and the eigenvector, is now

$$K(E) = d |\langle \lambda | E \rangle|^2 \\ = d \{ t^2 |\langle \lambda | R \rangle|^2 + (1-t^2) |\langle \lambda | I \rangle|^2 \}.$$

The invariance of $\{H_a\}$ under orthogonal transformations insures that, for fixed t and asymptotic d , the overlaps $\langle \lambda | R \rangle$ and $\langle \lambda | I \rangle$ vary across the ensemble as independent Gaussian random variables. Introducing $\rho_K(z)$ and $\rho_\theta(u)$ as the ensemble probability densities for $K(E)$ and $\theta = 4t^2(1-t^2)$, and $\rho_K(z|u)$ as the $\theta = u$ conditional strength density, we have $\rho_K(z) = \int \rho_K(z|u) \rho_\theta(u) du$. We find then, with I_0 a modified Bessel function, that

$$\rho_K(z|u) = u^{-1/2} e^{-(z/u)} I_0((1-u)^{1/2} z/u). \quad (4)$$

Monte Carlo calculations have shown that the first-moment approximation (exact for $\Lambda = 0, \infty$), $\rho_K(z) \rightarrow \rho_K(z|\bar{\theta})$, is more than adequate for the data analysis. To evaluate $\bar{\theta}$, the first moment of ρ_θ , we use first-order (renormalized) perturbation theory, including degenerate theory for nearest neighbors, to expand the H_a eigenstate in the H_0 -diagonal basis. $\bar{\theta}$ then appears in terms of an inverse-square energy-weighted sum with a damping term to take account of near degeneracies. The final result, exact to order Λ , turns out to be $3\bar{\theta} = 2\pi^2 \Lambda [2 - \gamma - \ln(2\pi^2 \Lambda)]$, good for $\Lambda^{1/2} \lesssim 0.2$.

For the strength bounds the data come from a major subset of the neutron-resonance sequences used for the spectral case,^{2,9} essentially groups 1-3 of Table I in Ref. 2. We combine sequences in the same group after renormalizing the strengths to unit means. Since the χ_1^2 and χ_2^2 forms differ most significantly for small arguments, our main interest is in the small strengths. It is good therefore to consider as a measure the distribution function $F(x; \epsilon)$, the density integrated from ϵ to x , for which the sample error from p strengths is $\{F(x; \epsilon)[1 - F(x; \epsilon)]/p\}^{1/2}$. Our analysis shows that the data for groups 2,3 agree with GOE for all $x \geq \epsilon$ if we choose $\epsilon = 0.004$; this choice of ϵ as a cutoff is dictated by the fact that very few levels with strengths $\leq \epsilon$ have been

observed. The optimal measure (which depends on the number of strengths) turns out to lie between $F(0.02; 0.004)$ and $F(0.07; 0.004)$ for all groups. Proceeding as in the spectral analysis with a 3σ confidence criterion we find that the $\Lambda^{1/2}$ bounds for groups 2 and 3 are essentially identical (0.17, 0.07) with the spectral bounds; uncertainties about the data prevent us at present from giving a bound for the first group. If an $\epsilon = 0$ cutoff had been appropriate the strength bound would have been smaller by a factor of 4.

The GOE ($\Lambda = 0$) strength analysis would suggest that a subset of the levels, randomly ordered in energy, is missing, the expected fraction being 5%, whereas the GOE spectral analysis would give essentially zero. A detailed analysis shows that consistency of these fractions has a low ($\lesssim 10^{-3}$) probability. They can, however, be reconciled by the assumption of a nonzero Λ , the optimal value, with expected fraction $\approx 1.5\%$, being $\Lambda^{1/2} \approx 0.03$ which is properly less than the derived bounds. Three possible explanations for the nonzero effective Λ are errors in the data, small-strength departures from the statistical model, and the actual occurrence of TRI breaking. It would not be prudent at this time to argue that the symmetry breaking has been observed.

For the $\Lambda \rightarrow \alpha$ reduction we observe that, while the Λ/α^2 values above are for individual nuclei, the Λ bounds² come from groups of nuclei, the grouping being by their complexity as displayed by D and being necessary to obtain adequate sample size. The resultant spectral α bounds are $\alpha_{sp} \leq (2.9, 3.3, 1.5, 2.6, 0.6) \times 10^{-3}$, the ordering being as given for Λ/α^2 above. The strength bounds are $\alpha_{st} \leq (2.8, 2.6, \dots, \dots) \times 10^{-3}$. It seems proper to quote, as the final bound for the relative norm of the TRNI nucleon-nucleon interaction, $\alpha \leq (1-2) \times 10^{-3}$. If we were to take seriously, as a measurement of TRNI, the value (for the combined data) derived from reconciliation of the data, the α value, e.g., for ²³³Th, would be 3×10^{-4} . It should be clear that to improve the α bounds (or even the values) we need more information about small strengths in complex nuclei, i.e., nuclei with small average spacings such as ²³⁶U. For a theoretical review of CP violation see Wolfenstein.¹⁰

We have stressed the generality of our solution to the $\Lambda \leftrightarrow \alpha$ problem. The generality of the Λ theory follows from its appearance as the "time" variable in a set of hierarchic equations¹¹ for the n -level correlation functions. This derives in turn from Dyson's diffusion equation¹² for the joint probability distribution of the eigenvalues, with α^2 as time and β^{-1} as temperature, by use of a renormalization process to eliminate the effects of distant levels. Dyson's equation applies specifically to the ensembles $\{H_a = H + \alpha U\}$ where $\{U\}$ in H -diagonal basis is a classical ensemble G_β , respectively GOE, Gaussian unitary ensemble (GUE), Gaussian symplectic ensemble (GSE) for $\beta = 1, 2, 4$. However the renormalization process is of such generality that the hierarchic set should apply to any $\{H_a\}$ in which $\{U\}$, in H -diagonal

basis, is *locally* G_β . For finite Λ , approximate² and complete¹³ solutions are available for $\text{GOE} \rightarrow \text{GUE}$ as well as $\text{GSE} \rightarrow \text{GUE}$. For the important Poisson $\rightarrow G_\beta$ transitions (relevant,¹⁴ e.g., with $\beta=1$, for atomic L, S symmetries) the small- Λ solution gives, for the number variance,⁷

$$\Sigma^2(r; \Lambda) \rightarrow \Sigma^2(r; 0) - 2\beta\Lambda \{\ln(r^2/2\Lambda) - \psi(\beta/2 + 1) + 1\}$$

with ψ the digamma function.

Since the classical ensembles involve only multibody interactions, it is important to ask whether the equations extend to the embedded ensembles defined above. There are strong theoretical arguments and experimental indications that the local- G_β assumption is valid for these ensembles. Then the above $\{H_\omega\}$, involving a realistic Hamiltonian, when embedded⁴ in m -particle spaces, should yield the same results for all $m \geq p > 1$ even though the global invariance of $\{U\}$ is lost for $m > p$. The NIP case, $m > p = 1$, is exceptional (physically because level crossing is not forbidden); for example, with H also NIP, it is described by the same equations with $\beta \rightarrow 0$, the large- Λ solution being then Poisson. This many-particle behavior is consistent with recent numerical and semiclassical theoretical results¹⁵ for systems with few degrees of freedom, not surprising since NIP relates to an integrable classical system and interacting particles almost always, to a chaotic one.

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