Spectroscopy with random and displaced random ensembles

V. Velázquez and A. P. Zuker

IRES, Bât27, IN2P3-CNRS/Université Louis Pasteur BP 28, F-67037 Strasbourg Cedex 2, France (December 28, 2002)

Due to the time reversal invariance of the angular momentum operator \( J^2 \), the average energies and variances at fixed \( J \) for random two-body Hamiltonians exhibit odd-even-\( J \) staggering, that may be especially strong for \( J = 0 \). It is shown that upon ensemble averaging over random runs, this behaviour is reflected in the yrast states. Displaced (attractive) random ensembles lead to rotational spectra with strongly enhanced \( BE2 \) transitions for a certain class of model spaces. It is explained how to generalize these results to other forms of collectivity.

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Even-even nuclei are more bound than their odd neighbours (OES, odd-even staggering). Their ground states have always spin \( J = 0 \) (J0D, \( J = 0 \) dominance), and with exceedingly few exceptions their first excited state has \( J = 2 \) and decays through an enhanced \( BE2 \) transition. These systematic features have been traditionally interpreted in terms of specific components of the nuclear interaction. OES, for instance was attributed to the pairing force but it has been argued that, in small Fermi systems, it is a universal phenomenon associated with deformation [1]. Though the claim is too strong, there is some truth in it as it can be viewed as a consequence of the Jahn-Teller effect which produces OES.

The discovery that random interactions lead to ground and \( J = 2 \) first excited states far more often than statistically expected \( [3] \) has brought the subject of systematic features into sharper focus. In particular, OES is often present, even in the absence of either pairing forces or deformed fields \( [2] \), which means that it should not be associated to a specific form of coherence. We are left to find general causes.

In what follows it will be argued that time reversal (\( T \)) invariance is at the origin of such behavior, as we shall see soon. The paradox is resolved by noting that the \( J^2 \) operator is \( T \) invariant, and states of good \( J \), transform as \( T | JM \rangle = (−)^{J+M} | J − M \rangle \) \( [4] \).

At \( M = 0 \), which contains the information on all states, eigenstates of \( J^2 \) are also eigenstates of \( T \), with eigenvalue \( (−)^J \): true for TBRE derived from GOE Hamiltonians are \( T \)-invariant, while those derived from GUE ones are not [2].

In Ref. [2] it was found that both ensembles lead to the same behaviour for OES and J0D. At first sight the result is surprising since \( T \) invariance is at the origin of such behavior, as we shall see soon. The paradox is resolved by noting that the \( J^2 \) operator is \( T \) invariant, and states of good \( J \), transform as \( T | JM \rangle = (−)^{J+M} | J − M \rangle \) \( [5] \).

The \( W^J_{rstu} \) matrix elements will be taken to belong to the Gaussian orthogonal ensemble (GOE), i.e., to be real and normally distributed with mean zero and variance \( \sigma^2 \) for the off-diagonals and \( 2\sigma^2 \) for the diagonals. For \( n > 2 \) the Hamiltonian matrices are said to belong to the two body random ensemble (TBRE). An alternative should be considered: GUE, where \( U \) stands for unitary, in which case the matrix elements are complex (general Hermitian, rather than symmetric, matrices). TBRE derived from GOE Hamiltonians are \( T \)-invariant, while those derived from GUE ones are not [6].

In a determinantal basis, at \( M = 0 \), if a state and its time reversed are different, the resulting even and odd states \( | jm j − m \rangle \) contribute equally to the traces of \( H^K \). The self conjugate states are always even \( (e.g., | jm j − m \rangle ) \). Therefore, at fixed number of particles \( n \) there are always more even \( J \) states than odd ones.

Obviously, the difference in average energies between even and odd states, \( \zeta \), will depend on the sign for the average over selconjugate states. Upon ensemble averaging \( \zeta \) will vanish, and we expect no staggering between \( E_{r,J} \) even and odd states. It is equally obvious that for the variances all contributions are positive. Hence the average \( \sigma^2 \) will always be larger for even states than for odd ones, and staggering will persist after ensemble averaging.

For odd \( n \), \( T \) has no consequences because it has no eigenstates: since \( T^2 = −1 \), the \( (1 ± T) | JM \rangle \) combinations change sign under \( T \).
To (try to) explain J0D we note that all the $J = 0$ states of seniority zero are in the self-conjugate space. It is fairly simple to calculate their centroids and widths. If they contribute substantially to the totals, much of the $J$-OES will be due to them and they will concentrate on the overall $J = 0$ averages thus explaining their special status. A strong hint in favor of this argument is the massive presence of seniority zero states indicated by the persistence of pair-transfer coherence in $J = 0$ ground states. To sum up all the indications related to $T$:

Whatever separates even and odd $J$ is due to the self-conjugate space, and whatever is special about $J = 0$ is due to the seniority zero states, entirely contained in this space. And, remember, $T$ invariance does not imply J0D, it only suggests its frequent observation.

The next task is to prove that $E_{cJ}$ and $\sigma_J$ are sufficient to determine the ensemble averaged yrst patterns. The proof is as follows: The low moments of $H$ determine a smooth tridiagonal matrix. Once diagonalized it leads to a smooth binomial that describes very well the level densities. The position of the yrst state depends on the parameter $N_J = \ln d_J / \ln 2$. If the third moment vanishes—as assumed here—the energy converges to the lower bound $E_{bJ} = E_{cJ} - \sqrt{N_J} \sigma_J^2$. For moderate values of $N_J$ ($\approx 10$ in our example) this limit is missed by $\approx 2\sigma_J / \sqrt{N_J}$ and a good estimate demands explicit diagonalization, which will obviously reflect $J$-OES.

This result is strictly true for ensemble averages. For individual matrices, because of fluctuations, the bound is only an unreliable estimate (an old story under a new guise). For example: with KB3, in $^{48}$Ca the $J \neq 0$ yrst states come below their exact positions by 0.25 to 2.5 MeV, while the ground state comes 4 MeV too high.

The subject demands a full treatment, but the arguments above are sufficient to confirm the crucial role of $\sigma_J$ anticipated in [7] but ignored in [4], and put in doubt in [7] through a misunderstanding that deserves a comment: Boson simulations are conducted in a collective subspace of much smaller dimensions than the corresponding fermion problem. In particular, the $N_J \times N_J$ tridiagonals in [7] (once corrected [8]) are interesting models for the Lanczos submatrix at the origin, but it makes no sense to compare their variance to that of the full $d_J \times d_J$ matrix ($d_J = 2^{N_J}$).

Of the three general properties mentioned in the first paragraph, BE2 enhancement is the one not spontaneously produced by purely random trials. Some coherence is needed, and the only way to simulate it, in a GOE context, is through a constant displacement, $c$, of all matrix elements. The displaced GOE (DGOE) is a standard ensemble, for which there exists a famous result: its spectrum is a semicircle, with one detached level [9]. Therefore, for attractive forces, the coherent part is a matrix whose elements are constants $c = -|c|$; leading to a displaced TBRE (DTBRE).

In a two-body context with good $J$, attractive forces do not have systematically negative matrix elements, but their signs must have a very general origin, because all realistic interactions are spectacularly similar [10], and the extremely rare sign discrepancies only affect the smallest absolute values. Furthermore, as was noted in Ref. [9], these signs are strongly correlated to those of Elliott’s $q \cdot q$ force. Hence, there may be a—DTBRE vs $q \cdot q$—“sign coherence” conflict.

Quite conveniently, it is possible to analyze—and then resolve—it, while staying within the DTBRE; by examining results in two spaces. The first is a ($\Delta J = 2$) subspace of a major shell, in which all $q \cdot q$ and realistic matrix elements are negative. It consists of the orbits with $j = l + 1/2$, for which a quasi-SU3 symmetry can

![FIG. 1. ($pf)^{8,9}$ centroids and widths. See text](image-url)
operate, leading to quadrupole properties similar to those of the full shell \[29\]. The second is the major shell itself.

Accordingly, two sets of runs were performed. The first in the \(\Delta J = 2\), \((J_{f/2}/p_{3/2})\) space (\(fp\) for short) respects sign coherence. The other, in the full \(pf\) shell, does not. **Please do not confuse \(fp\) and \(pf\).**

960 \(fp\) runs were done for each of four combinations of number of particles and isospin: \(nT = 84\) (\(^{48}\text{Ca}\)), 40 (\(^{44}\text{Ti}\)), 61 (\(^{46}\text{Ti}\)), and 80 (\(^{48}\text{Cr}\)), with strict GOE interactions plus single particle splitting. The parameters were chosen to mock realistic values (\(\nu = 0.6\), \(\epsilon_{f_{3/2}} - \epsilon_{p_{1/2}} = 2\) MeV). The \(c = -1\) steps for DTBRE are arbitrary.

Fig. 2 shows the evolution as a function of \(c\) of the \(R = E_4/E_2\) energy ratio, a time-honored indicator of collective behaviour: \(R = 1, 2, 3.33\) corresponding to seniority, vibrational and rotational regimes respectively. The discrepancies can be summed up by saying that in the full \(pf\) shell nothing is as clearcut as in the \(fp\) space, especially the limiting behavior for large displacements.

The situation at \(c = -2\) is typical. In the \(pf\) runs we find “only” 75% of \(J = 0\) ground states (against 99.8% in \(fp\)), and practically as many perfect sequences. The indicators are good—but more spread than in Figs. 2 and 3—at \(E_4/E_2 = 2.92 \pm 0.56\) and \(BE_2(2 \rightarrow 0) = 276 \pm 28\) \(e^2 fm^4\) (the \(SU3\) limit is 320 \(e^2 fm^4\), the strength is equally large in \(J \neq 0\) ground states). More disturbingly, the runs do not seem to converge to perfect rotors: \(c = -3\) brings little change over \(c = -2\). The fairly good rotational behaviour suggested by the averages above is not systematically confirmed by a well defined intrinsic state. In other words: \(Q_0\) is not always approximately constant for the lowest members of the band. In the \(fp\) case, at \(c = -2\), 99.8% of the sequences are perfect and all yrast levels are those of a rotor.

Statistically, sign-coherence is not indispensable to generate acceptable \(BE2\) enhancements, but physically it matters: Even nuclei do not have \(J = 0\) ground states 50 or 80% of the time, but 100% of the time.

| \(c\)  | \(^{48}\text{Ca}\) | \(^{44}\text{Ti}\) | \(^{46}\text{Ti}\) | \(^{48}\text{Cr}\) |
|---|---|---|---|---|
| 0  | 76.3 | 46.6 | 33.2 | 60.2 |
| -1 | 72.8 | 59.4 | 65.0 | 88.1 |
| -2 | 61.1 | 82.0 | 94.9 | 99.8 |
| -3 | 53.3 | 94.7 | 99.7 | 100.0 |

**TABLE I.** Percentage of \(J = 0\) ground states as a function of displacement \(c\).
$^{48}$Cr has better than 75% chances of having a rotational-like behaviour: it is a backbending rotor.

Fig. 4 illustrates what a constant interaction $W_{rstu}^{JT} = -a$ does in the $\Delta J = 2, (gds)^8 T = 0$ space. With single particle spacings of 1 MeV, the $E_{J+2} - E_J$ patterns are those of backbending rotors. They show more structure than the realistic interaction results [20] but the physics is very much the same.

![Backbending patterns in $(gds)^8 T = 0$, with KLS interaction from [20], and constant $W_{rstu}^{JT} = -a$.](image)

At this point, as far as DTBRE in the $pf$ shell goes, we are where we were twenty years ago in the $sd$ shell: The $BE2$ coherence is there but “The spectra are neither rotational nor particularly interesting” [19]. But now we have the $fp$ spectra: rotational, and therefore interesting. The difference is obviously due to sign-coherence. But: Why do we have sign-coherence in $fp$? Because in $\Delta J = 2$ spaces, the signs, by construction, are the same as in $LS$ coupling [21].

The heart of the problem is that we do, routinely, simulations in $jj$ coupling because it is the one used in shell model codes, as commanded by the central—more generally monopole—field. However, the “residual” two body multipole part of the Hamiltonian is dominated by forces that are overwhelmingly central (quadrupole, pairing, etc.) [1]. For these, the natural coupling scheme is $LS$. Therefore, it is artificial to define for them DTBRE coherence through the $jj$ matrix elements.

The solution of the sign-coherence problem becomes evident: define the DTBRE in $LS$ scheme. Technically, we can continue to employ $jj$ scheme using the $LS$ displacement calculated once and for all. It is a safe bet—backed by the $sd$ experience [19]—that the $pf$ results will become as satisfactory as the $fp$ ones.

Our examples involve rotational motion, but now it should be possible to generate other forms of collectivity, as seen by the simplest example: with the same two body interaction the $(sd)^4$ spectrum is rotational ($^{20}$Ne) and the $(sd)^{-4}$ spectrum is vibrational ($^{36}$Ar). The difference between the two is entirely due to the change of central field. Therefore, to obtain both rotors and vibrators it seems convenient to randomize the single particle energies and fix the two body terms, contrary to what is usually done.

We have identified time reversal invariance as the origin of odd-even staggering of the mass surfaces and $J = 0$ spin for the ground states of even nuclei. The attractive nature of the forces appears to provide a sufficient condition $BE2(2 \to 0)$ enhancements associated to collective behaviour.

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