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WIGNER MODEL AND REAL ATOMS: AN EXAMPLE

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НОВОСИБИРСК

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Abstract

Comparison of the Wigner BRM model with a series 4^+ eigenstates in Cerium atom is considered. It is shown that such a generic model provides a satisfactory description of the global structure of chaotic atomic states. Several improvements are suggested to incorporate into the model some more realistic atomic features like a smooth matrix band and its sparsity.

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The first attempt to describe statistical properties of complex quantum systems by means of random matrices goes back to Wigner [1]. He introduced a Band Random Matrix (BRM) model to describe conservative systems like atomic nuclei [2]. Specifically, he considered an ensemble of real, infinite, Hamiltonian matrices of the type

$$H_{mn} = \frac{m}{\rho}\delta_{mn} + v_{mn}\,, \qquad v_{mn} = v_{nm} \tag{1}$$

where ρ is the mean level density; the off-diagonal matrix elements are random and statistically independent with $< v_{mn} >= 0$ and $< v_{mn}^2 >= v^2$ for $|m-n| < b$, while $v_{mn} = 0$ otherwise; b is the band width.

Wigner introduced also the weighted level density

$$w_{GS}(E;\,m) = \sum_l a_{ml}^2\,\delta(E - E_l) \tag{2}$$

where a_{ml} are components of the eigenfunctions ψ_l of Hamiltonian (1) in some physically significant unperturbed basis $\{\varphi_m\}$, and E_l are eigenvalues corresponding to ψ_l.

The density $w_{GS}(E;\, m)$, called *strength function* by Wigner (the term still in use in nuclear physics), proved to be very important in the studies of quantum statistics, and is now called also *local spectral density* (see, e.g., Ref.[3]). It is related to the so–called *operative eigenfunctions* [4] which actually control the dynamics of the initial state φ_m. Hence still another term for w_{GS}, the *Green spectrum* we now use [5].

The analytical evaluation of the density (2) turned out to be very difficult. Only in two limit cases Wigner was able to derive an explicit expression for w_{GS}, namely: for the semicircle ($q = (\rho v)^2/b \gg 1$), and for Breit - Wigner laws (for recent development see Ref.[6]).

After Wigner's pioneering work, BRM were almost forgotten (curiously enough by Wigner himself [7]), apparently because of their mathematical inconvenience, namely, non-invariance with respect to basis rotation. Due to this, attention was paid mainly to full random matrices for which a fairly complete mathematical analysis has been developed [8]. However, full random Hamiltonian matrices can be used to describe the local statistical properties only, the restriction which is especially bad for atoms [9].

A physically meaningful approach to the analysis of global properties of Hamiltonian systems can be obtained by just going back to the original Wigner model with increasing diagonal elements (1). In this model the semicircle law holds for the weighted level density (2) only, while the total level density is approximately uniform in the semiclassical region. Moreover, in physical applications, the interaction of unperturbed states always has a finite range which determines the band structure of Hamiltonian matrices. For this reason, there has been a revival of interest in BRM [10]. Particulary, in Refs.[11] the energy level statistics has been studied in the original Wigner model (1).

To which extent a relatively simple Wigner model does represent a real physical system?

Below, we discuss this important question using as an example the series $J^\pi = 4^+$ of about 100 excited eigenstates in the Cerium atom which was studied in detail in Refs.[12, 13] following Ref.[9] where the global structure of chaotic atomic eigenstates had been first estimated.[1] The average energy of the Ce states is about 3 eV above the ground state as compared to 5.54 eV for the ionization threshold. The main parameters of the corresponding matrix were found to be as follows: $\rho = 31\ eV^{-1}$; $v = 0.1\ eV$; $b = 100$ for the matrix size $N = 276$ which is a technical parameter in the Wigner model (see Ref.[5] for details). It makes the Wigner parameter $q = 0.1$ which corresponds to the structure of the energy shell intermediate between Breit - Wigner's and semicircle's one (Fig.1). As a result there is some uncertainty in evaluation of the ergodicity parameter [5]: $\lambda_{SC} \approx 70$; $\lambda_{BW} \approx 50$. However, the result is clear in that the eigenfunctions must be very close to *ergodic* contrary to the conclusion in Ref.[18] where the same example was discussed.

The shape of the average eigenfunction is shown in Fig.1 by squares. The averaging was made in two steps: first, within each of 6 groups of close 19 eigenstates, and second, by superimposing of the maxima of these groups. Whether the structure emerging upon averaging is of a physical origin or is some residual fluctuations remains unclear. To our knowledge, this is the first example of the real chaotic eigenstates, and not only in atoms but also in nuclei. Before, only Green spectra were studied whose structure is generally different from that of eigenfunctions [5].

At the first glance, the shape of atomic eigenfunctions looks rather different as compared to that in the Wigner model. There are, at least, two striking differences:

[1] This first estimate was based essentially on the data of many laboratory experiments as summarized in [19]. Unlike this, a much more detailed structure of atomic states presented in [12, 13] was calculated numerically using new powerful techniques. Even though some doubt as to the accuracy of the latter data might still exist the statistical properties of atomic eigenstates we only need here appear to be fairly reliable.

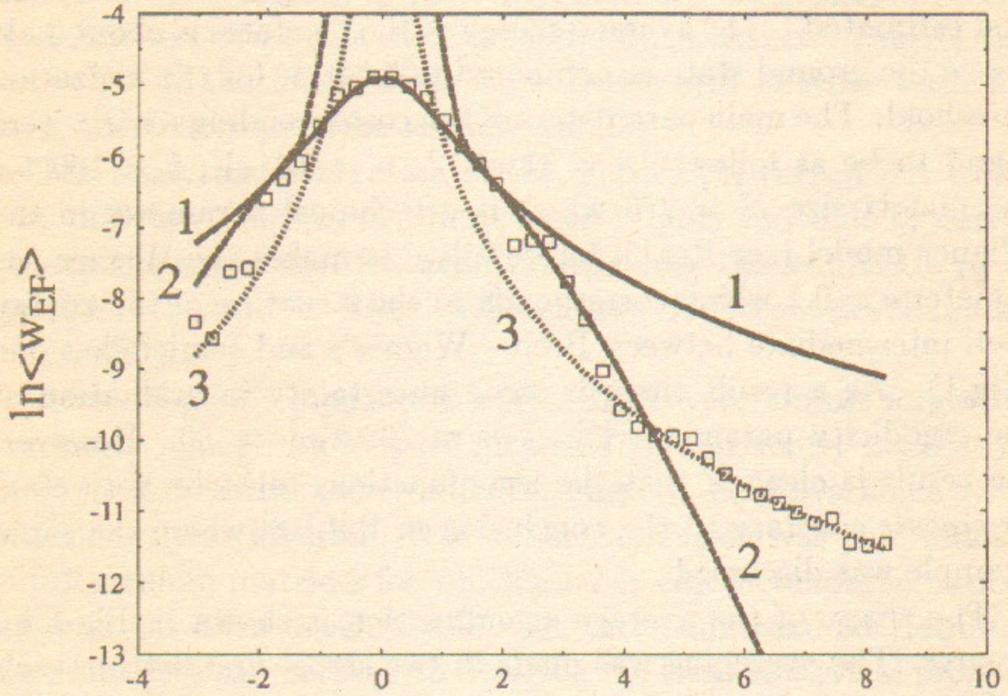

Figure 1: The average eigenfunction of Cerium atom from 19×6 individual eigenfunctions 4^+ [12] (squares): $w_{EF} = |\psi_{EF}|^2$ is the eigenfunction probability (arbitrary units) for the basis states of energy E in eV. Solid line 1 is the Breit - Wigner distribution (3) with fitted $\Gamma \approx 2\ eV$; dashed line 2 is the Wigner tail (4) with fitted $b \approx 100$; dotted line 3 is direct coupling (5) with a fitted power–law tail (6) of the Hamiltonian matrix in Fig.2.

(i) the distribution is rather asymmetric with respect to the maximum, and

(ii) there is additional slow–decaying tail on the right.

The first peculiarity is apparently related to a short basis. However, it cannot be extended to the left as the leftmost basis states are already close to the ground state. Surprisingly, the upper part of the distribution remains approximately symmetric with respect to the maximum.

The eigenfunction cap is well represented by the Breit - Wigner law:

$$w_{EF} = \frac{w_m}{\epsilon^2 + (\Gamma/2)^2}, \quad \epsilon = E - E_0 < \frac{b}{\rho} \tag{3}$$

with fitted $w_m = 7.55 \times 10^{-3}$ and $\Gamma/2 \approx 1\ eV$ which is close to $\Gamma/2 \approx 0.9\ eV$ in Refs.[12, 13]. However, a characteristic Breit - Wigner tail is absent because of a low cut–off at $b/\rho \approx 3.3\ eV$. Instead, the Wigner tail (corrected in Ref.[12], see also Ref.[16]) shows up:

$$\ln w_{EF} \approx A - \xi\,[\ln(\zeta \cdot \ln\zeta) - 1.6] \tag{4}$$

where $\xi = \rho\epsilon/b$, $\zeta = \xi^2/q$, and fitted $A = -6.49$. This simple relation approximately describes the eigenfunction down to $E \approx 1.5\ eV$, much lower the cut–off energy. Moreover, two curves, (1) and (2), are tangential at the intersection [12] which is not the case generally[6].

We used Eq.(4) for evaluation of the effective band width $b \approx 100$. However, the fine structure and/or residual fluctuations in the average eigenfunction as well as the narrow energy interval $(1.5 - 4.5\ eV)$ for the Wigner tail substantially restrict the accuracy of b value. The discrepancy with $b \approx 80$ in Ref.[12], obtained by a different method, characterizes a real accuracy which is not so bad for a rather crude approximation of the real Hamiltonian matrix by a simple one in generalized Wigner model (Fig.2).

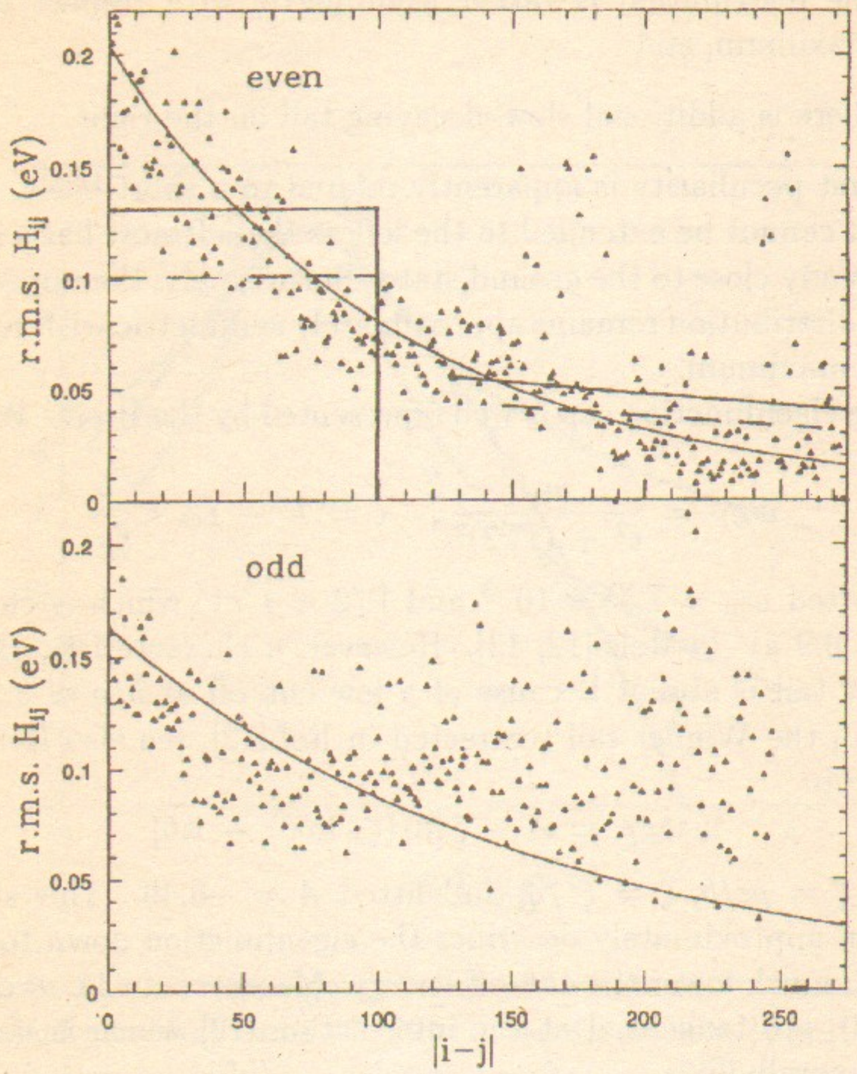

Figure 2: Distribution of matrix elements (solid triangles, upper half) fitted by the exponential (solid curve) [13], and a crude approximation in generalized Wigner model: upper solid lines represent the main part of model's Hamiltonian with $v_0 \approx 0.13\ eV$, $b = 100$, and the tail (6) with sparsity $s_0 = 0.6$ and $p_H = 0.4$; lower dashed lines give recalculated values of $v = v_0\sqrt{s_0}$ corresponding to $s = 1$ (cf. Ref.[6]).

The additional tail on the right was fitted by a power law:

$$w = \frac{c}{\epsilon^p} \tag{5}$$

with $c = 3.2 \times 10^{-3}$, and $p = 2.73$. Our attempts to fit the tail to any reasonable exponential failed.

The physical mechanism of the tail formation is apparently related to the direct coupling of far basis states due to a long tail in the Hamiltonian matrix itself (Fig.2). However, it would imply, in the first–order perturbation theory, a very slow decay of the matrix elements:

$$H_{ij} \approx \frac{0.25}{|i-j|^{p_H}}, \quad |i-j| \gtrsim 130 \tag{6}$$

with $p_H \approx 0.37$ which seems to be very difficult to agree with the actual decay in Fig.2 in spite of big fluctuations. A possible explanation of this apparent discrepancy is in that the asymptotic behavior (6) is not yet reached in the range $4 - 8\ eV$ (Fig.1), and higher orders of perturbation theory are required.

Localization length (Hilbert dimension) of the average eigenfunction was found to be $d_P = 126$ (from the participation ratio, see, e.g., Ref.[14]). In the semicircle approximation the ergodic dimension were $d_e = 157$. A better agreement is achieved by using the Wigner model with $q = 0.1$ as in the Cerium atom: $d_e = 140$. Remaining discrepancy ($\approx 10\%$ assuming ergodicity) is again not that bad. Particularly, it is related to a physically restricted basis: the ratio $N/d_e \approx 2$ is certainly not sufficiently large. The ergodicity of the Ce eigenfunctions can be directly measured using the methods proposed in Ref.[5], for instance, by computing the Hilbert dimensions of the Green spectra which must be the same in case of ergodicity.

A relatively small Hilbert dimension $d_e \approx 130$ emphasizes the importamce of the global structure in atoms [9] as compared to

nuclei where $d_e \sim 10^6$! The origin of such a big difference for comparable quantum numbers is not completely clear. Apparently, it is related somehow to an additional independent fermion in nuclei (proton and neutron as compared to electron in atoms).

The above comparison of relatively simple (but far from theoretically analysed!) Wigner model with a real physical system suggests already some immediate improvements of the model without loosing its generic nature (cf. more specific matrix models like one in Ref.[15]):

- a smooth distribution of matrix elements across the band (Fig.2) which has been already taken into account, at least formally, in Refs.[6, 16], and which was included roughly in the above theoretical analysis;
- a variation of matrix parameters ρ, v, b within the energy shell (Fig.1), also considered in Ref.[16];
- a finite size N of the physical basis which is not always a 'technical' parameter as in the original Wigner model;
- the sparsity of the Hamiltonian matrix which crucially depends on the basis chosen; for example, in Ref.[12] two bases are considered with sparsity (the fraction of nonzero matrix elements) $s = 0.6$ (discussed above), and $s = 0.06$ (!) only.

Including sparsity must be done with some care as follows from Ref.[17]. Taken literally, $s \to 0$ with increasing quantum numbers in the quasiclassical region. The difficulty is in that the remaining nonzero matrix elements are strongly correlated and cannot be considered as random in any sense. This is a typical situation as the original perturbation in a physical system is usually a simple and fairly regular function, the dynamical chaos being developed as a result of the action of such a perturbation. One possible solution of this difficulty is in constructing the unitary

matrix (a map) instead of the Hamiltonian one. However, increasing diagonal matrix elements (finite level density ρ), which is the most important property of the Wigner model for describing conservative systems, is lost, and it is not clear how to restore it. A more simple method seems to be in variation of the basis in such a way to keep sparsity, at least, constant (with increasing quantum numbers) and not too small.

In conclusion we would like to emphasize again that using random matrices (even a single matrix!) considerably simplifies both numerical experiments as well as the theoretical analysis without loosing essential part of the dynamical properties of real physical systems.

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