Band structure of the Hamiltonian matrix of a real "chaotic" system: The Ce atom

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The properties and structure of the Hamiltonian matrix of a realistic many-body quantum chaotic system (the rare-earth atom of Ce) are analyzed and compared with those assumed in band random matrix theories. The sparsity of the matrix and the behavior of the mean squared matrix elements $\langle H_{ij}^2\rangle_{|i-j|=\Delta}$ as function of the distance $|i-j|$ from the diagonal are studied. Fitting $\langle H_{ij}^2\rangle_{|i-j|=\Delta}$ with the exponent $H_0^2\exp(-\Delta/b)$ yields the bandwidths of b =54 and 79 for the matrices of $J^\pi = 4^+$, and 4^- states, respectively.

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It was shown in our previous work [1] that the rare-earth atom of Ce is an interesting example of a real quantum chaotic system. The aim of the present work is to study the structure and properties of the underlying Hamiltonian matrix of this problem. It is very instructive to compare them with those hypothetically stipulated in various random matrix models. This may also give some "experimental" foundations for such models.

After the pioneering works by Wigner [2] the random matrix theory (RMT) developed into a powerful instrument for studying statistical properties of spectra of complex quantum systems. Most progress in RMT was achieved for full random matrices, e.g., those of the Gaussian orthogonal ensemble, because of their invariance properties and relative mathematical simplicity of the problem (see review [3]). However, full random matrices account only for the local fluctuations and correlations in the spectrum and produce an unphysical semicircle spectral density of eigenvalues. The corresponding eigenstates are delocalized. It was probably this understanding that prompted Wigner [2] to suggest originally a band random matrix (BRM) model for describing complex atomic nuclei: $H_{ij} = 0$ if $|i-j| > b$, where b is the bandwidth.

Another essential feature of Wigner's model is the presence of a leading diagonal in the Hamiltonian matrix. It describes the increase of the basis state energies that takes place in any finite quantum system. The role of the diagonal is paramount, since the ratio of the typical off-diagonal matrix element to the average level spacing V/D determines the perturbative ($V/D < 1$), or nonperturbative ($V/D \geq 1$) and, possibly, chaotic character of the mixing of states. Recently BRM with a diffuse band have been considered with $\overline{H_{ij}^2}$ rapidly decreasing as a function of $|i-j|$ at $|i-j| \gtrsim b$. Localization properties of BRM were analyzed in [5] (see also [6], and references therein) and some analytical results for BRM without leading diagonal were obtained in [7,8].

It was shown in [4] that the banded structure of the Hamiltonian matrices emerges in the semiclassical regime. However, in many real systems such as the compound nuclei or rare-earth atoms the excitation energies are relatively low and the behavior of these systems is strictly quantum. Nevertheless, there are physical arguments that suggest bandedness of the corresponding Hamiltonian matrices. Indeed, consider the Hamiltonian matrix of a many-body system with a two-body interaction in the natural basis of many-particle states constructed from single-particle orbitals. In this basis only the matrix elements between states with no more than two different single-particle orbitals are nonzero. If two of the basis states are far apart on the energy scale the Hamiltonian matrix element coupling them involves distant single-particle states and is thus suppressed.

Although a lot of effort has been put into studying RM models, little is known about the structure of the Hamiltonian matrices of real systems that display quantum chaotic behavior. We believe that the present work contains the information one needs to construct a realistic BRM, and thus narrows the gap between RMT and real systems.

The electronic structure of the Ce atom is Xe-like, $1s^2\cdots 5p^6$ core with four valence electrons above it. The calculations are performed using the Hartree-Fock-Dirac (HFD) and configuration interaction (CI) methods [9]. The configurations of the valence electrons relativistic orbitals are built of $4f_{5/2}$, $4f_{7/2}$, $6s_{1/2}$, $5d_{3/2}$, $5d_{5/2}$, $6p_{1/2}$, and $6p_{3/2}$. Using the input list of the configurations of given parity, a basis containing all possible single-determinant states Ψ_i is constructed and the Hamiltonian matrix $H_{ik} = \langle\Psi_i|\hat{H}|\Psi_k\rangle$ in the single-determinant basis is evaluated. Since the eigenstates of the system are also eigenstates of the $\hat{J}^2$ operator, a new basis has been constructed (see [1] for details):

$$\Psi_{Ji} = \sum_{i'} A_{Ji,i'}\Psi_{i'} \ , \tag{1}$$

$$\hat{J}^2\Psi_{Ji} = J(J+1)\Psi_{Ji} \ ,$$

$$\langle\Psi_{J'i}|\hat{H}|\Psi_{Jk}\rangle = \sum_{i',k'} A^*_{J'i,i'}H_{i'k'}A_{Jk,k'} = H^{(J)}_{ik}\delta_{JJ'} \ , \tag{2}$$

where each Ψ_{Ji} is a linear combination of the single-determinant states belonging to one relativistic configuration, which possesses definite J. The Hamiltonian matrix constructed in this way has a block-diagonal structure and each block $H^{(J)}_{ik}$ is diagonalized separately. The new basis states Ψ_{Ji} are enumerated such that the diagonal matrix elements $H^{(J)}_{ii}$ increase with i. Below, as in [1], we consider $J^\pi = 4^+, 4^-$ states of the atom. For $J^\pi = 4^+$ the block contains $N = 276$ states and for $J^\pi = 4^-$ it has $N = 260$. In both cases the average spacing between $H^{(J)}_{ii}$ was $D \simeq 0.03$ eV.

In [1] we studied the probability densities of the off-diagonal matrix elements $H_{ij} \equiv H_{ij}^{(J)}$ (hereafter we drop the J index for convenience). The distributions for the even and odd matrices turned out to be very similar ([1], Fig. 10). We noticed that there is a large number of small matrix elements accumulated in the central bin and about 40% of them are zeros. This is explained by the fact that the matrix element between two configurations vanishes if they contain more than two different orbitals. There are also some approximate "nonrelativistic" selection rules due to conservation of the total orbital angular momentum L and the total spin S. These rules are violated by the spin-orbit interaction and they are "hidden" in the case when relativistic (nlj) orbitals are used. Nevertheless some basis states can have almost definite L and S values and give small matrix elements when L or S change. We showed that for larger H_{ij} the distribution is described well by a simple exponential fit

$$P(H_{ij}) \propto |H_{ij}|^{-1/2} \exp\left(-\frac{|H_{ij}|}{V}\right) , \qquad (3)$$

with $V = 0.12$ eV as the characteristic value of the off-diagonal matrix element. Using the distribution (3) one obtains the root-mean-square of $\sqrt{\overline{H_{ij}^2}} = \frac{\sqrt{3}}{2} V \simeq 0.104$ eV. This number is close to the root-mean-squared values of the nonzero off-diagonal matrix elements calculated directly for the even and odd matrices 0.114 and 0.113 eV, respectively.

The main feature of the off-diagonal matrix elements H_{ij} is that their dependence upon i and j is almost random. It occurs because the basis states belonging to different configurations are strongly interspersed on the energy scale, and the basis states Ψ_{Ji} themselves are rather complex linear combinations of simpler single-determinant states. In order to check whether there is any regular dependence of H_{ij} on i and j the *locally* averaged $\langle H^2 \rangle_{ij}$ were calculated in [1]:

$$\langle H^2 \rangle_{ij} = \frac{1}{(2W+1)^2} \sum_{\substack{|i'-i| \le W \\ |j'-j| \le W}} H_{i'j'}^2 , \qquad (4)$$

where we used $W = 9$. A clear feature of $\langle H^2 \rangle_{ij}$ as a function of i and j is the existence of a "craggy ridge" along the main diagonal ([1], Fig. 9), more pronounced for the even states matrix. This is an indication of a bandlike structure of the matrices. However, there are two effects that may contribute to such behavior of $\langle H^2 \rangle_{ij}$. Firstly, the matrix elements may indeed get smaller as $|i-j|$ increases. Secondly, the number of zero matrix elements may increase as we depart from the matrix diagonal. In other words, the matrix may be getting sparser.

In order to probe the bandlike structure of the Hamiltonian matrix we show in Fig. 1 the dependence of H_{ij} on their distance from the diagonal $\Delta = |i-j|$. One can see that the matrix elements H_{ij} indeed decrease as $|i-j|$ increases. Figure 2 presents the sparsity of the matrices for the even and odd states. The sparsity is defined for $|i-j| = \Delta$ as the ratio of the number of nonzero matrix elements (more precisely, $|H_{ij}| > 10^{-6}$ a.u. $\simeq 3 \times 10^{-5}$ eV) to the total number of matrix elements (according to

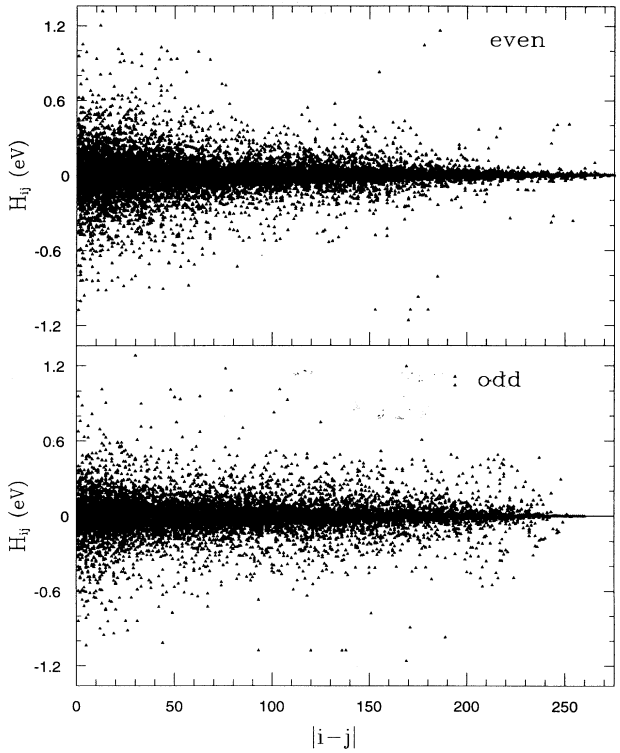

FIG. 1. Matrix elements H_{ij} (eV) presented as a function of the distance to the main diagonal $|i-j|$ for the even and odd states.

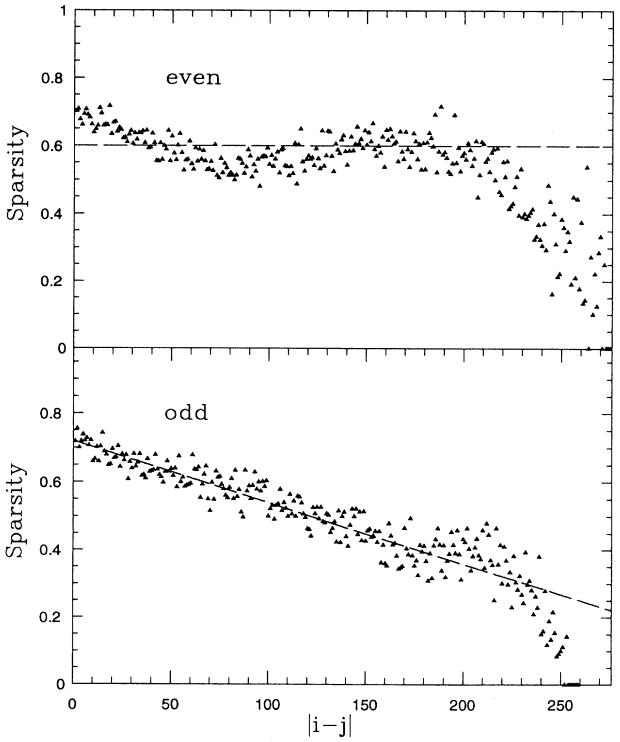

FIG. 2. Sparsity of the Hamiltonian matrix S = (number of $|H_{ij}| \neq 0$)/(number of all H_{ij}), $|i-j|$ fixed. Dashed line shows a linear approximation for S.

TABLE I. Quantitative characteristics of the sparsity and bandlike structure of the Hamiltonian matrices. The third column lists the mean-squared value of the nonzero off-diagonal matrix element. The fourth and fifth columns list the parameter for the fit of the matrix sparsity, $S(i-j) = S_0 - k|i-j|$. The sixth and seventh columns list the parameter of the fit $\langle H_{ij}^2 \rangle_{|i-j|=\Delta} = H_0^2 \exp(-|i-j|/b)$.

Levels	N	$\overline{H_{ij}^2}$ (eV^2)	S_0	k	H_0 (eV)	b
Even	276	0.0130	0.6	0	0.204	53.5
Odd	260	0.0128	0.72	0.0018	0.163	79.3

this definition the sparsity is 1 for full random matrices). The difference between the matrices is quite noticeable. In the case of even states the Hamiltonian matrix demonstrates almost constant sparsity, whereas in the case of odd states there is a clear linear decrease. Dashed lines show a linear approximation $S(\Delta) = S_0 - k\Delta$ for the sparsity in both cases. Parameters of the fit are given in Table I. The observed sparsities agree with an estimate made in [1] that nonzero matrix elements comprise about 60% of the matrices.

In order to estimate the bandwidth b we fit the mean squared matrix elements with a simple exponential ansatz (this analytic form was used in [8]):

$$\langle H_{ij}^2 \rangle_{|i-j|=\Delta} = H_0^2 \exp(-\Delta/b) \ , \qquad (5)$$

where $\langle H_{ij}^2 \rangle_{|i-j|=\Delta}$ is the average of the squared nonzero matrix elements at a given distance Δ from the diagonal. The dependence of $\langle H_{ij}^2 \rangle_{|i-j|=\Delta}$ on Δ for even and odd state matrices is shown in Fig. 3. The values of H_0 are chosen to describe the data in the vicinity of the main diagonal, i.e., for small $|i-j|$. If we express the overall mean square value of the nonzero matrix element in terms of the matrix sparsity and partial averages (5), the following equation must be fulfilled:

$$\frac{H_0^2 \int_0^N (S_0 - k\Delta)\ (N-\Delta)\ \exp(-\Delta/b)\ d\Delta}{\int_0^N (S_0 - k\Delta)\ (N-\Delta)\ d\Delta} = \overline{H_{ij}^2}, \qquad (6)$$

where $\overline{H_{ij}^2}$ is the average over all nonzero matrix elements in the Hamiltonian matrix. The values of b found from (6) are presented in Table I together with other numerical data involved in (6).

The values of b =53.5 and 79.3 have been obtained for the even and odd matrices, respectively. Both of these values are much smaller than N, which should clearly indicate the band structure of the matrices. However, one can see from Fig. 3 that while the fit (5) looks very reasonable for the even matrix, it is not quite relevant for the odd matrix. We should note that in both cases, especially for the odd matrix, there are distant basis states coupled by large matrix elements H_{ij} that do not obey (5). It implies that the Hamiltonian eigenstates must contain "small components": perturbation theory

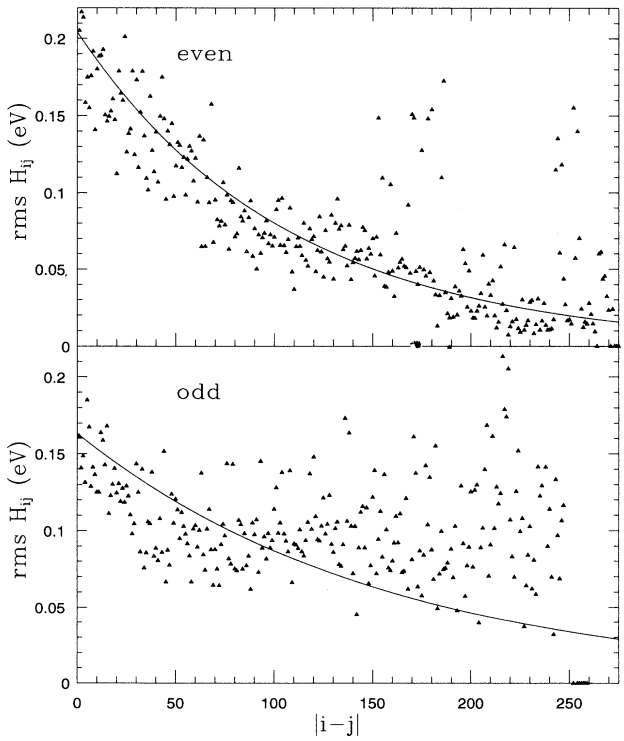

FIG. 3. Root-mean-squared matrix elements $\langle H_{ij}^2 \rangle_{|i-j|=\Delta}^{1/2}$ as a function of the distance to the main diagonal. Solid line shows the fit $\langle H_{ij}^2 \rangle_{|i-j|=\Delta}^{1/2} = H_0 \exp(-|i-j|/2b)$, where b is the bandwidth.

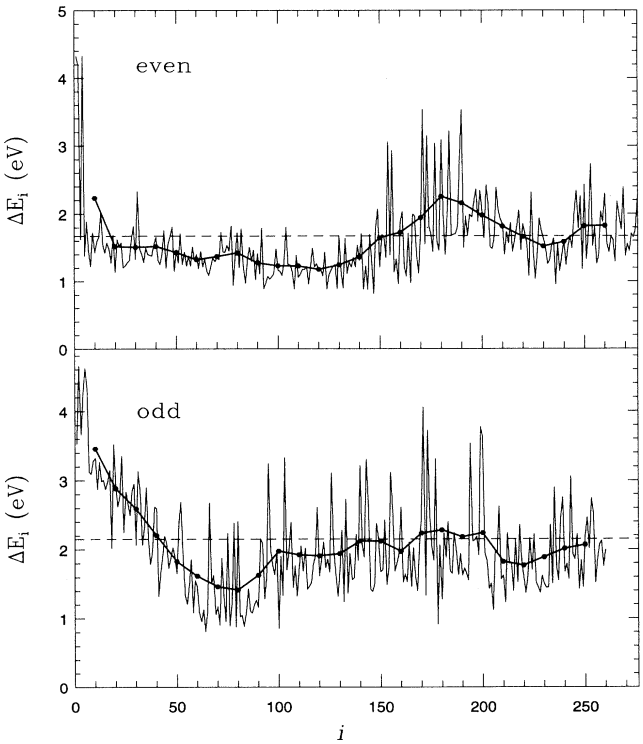

FIG. 4. Energy bandwidths ΔE_i for the even and odd matrices. Dots connected with a thick line show local root-mean-squared values $\sqrt{\langle \Delta E^2 \rangle_{i_0}}$ for $i_0 = 10, 20, \ldots$ averaged over $|i - i_0| \leq 9$. Dashed line is the overall root mean squared energy bandwidth (1.67 and 2.15 eV for the even and odd matrices, respectively).

contributions of the distant states (which cannot be described by BRM). Indeed, we observed those in [1] (Figs. 11, 12, and 20) as additional "bumps" in the strength functions of the states. In agreement with the difference between the even and odd matrices (Fig. 3) they manifested stronger for the odd eigenstates. We can compare the above bandwidths with a rough estimate made in [1]. If one assumes that all 60% of nonzero matrix elements are located within the band $|i-j| \leq b$, a value of $b \simeq 80$ is obtained.

In Fig. 4 we present the energy bandwidths calculated according to [4]

$$(\Delta E_i)^2 \equiv \frac{\sum_j (H_{ii}-H_{jj})^2 |H_{ij}|^2}{\sum_{j\neq i} |H_{ij}|^2} \ . \tag{7}$$

In both cases there are large fluctuations in ΔE_i, more noticeable for the odd matrix. Apart from them, the locally averaged energy bandwidth displays a relatively slow dependence on i, or, accordingly, on the excitation energy, within the 10-eV range studied. The root-mean-squared bandwidths of $\Delta E = 1.67$ eV (even) and $\Delta E = 2.15$ eV (odd) correspond to the number bandwidth $b = \Delta E/D \simeq 56$ and 72, respectively ($D \simeq 0.03$ eV). These values are quite close to those determined from Eqs. (5) and (6).

We believe that the energy bandwidth is a better and somewhat "more physical" characteristic of the Hamiltonian matrix, since it refers to the energy interval within which the perturbation strongly mixes the basis states. If, for instance, we defined b as $\Delta E/D$ using *locally averaged* ΔE and D, the result would show dramatic variations with energy. The point is that the level density $\rho(E) = D^{-1}$ in many-body systems strongly (exponentially) depends on the excitation energy (see, e.g., [10] for the level density in atomic Tb), thus producing a strong energy dependence of the number bandwidth b. Therefore, one can expect the values of ΔE to be similar for various systems of a particular class (say, for different atoms), whereas the magnitude of b will be quite different for them, depending on, e.g., the number of interacting particles (valence electrons).

Using the CI method we studied the Hamiltonian matrices of $J^\pi = 4^+, 4^-$ states of the rare-earth atom of Ce. It has been shown that these matrices can be characterized as sparse band matrices with the leading diagonal. Therefore, BRM models seem to be more relevant for describing real physical systems. However, there always exist some distant basis states strongly coupled by the residual interaction (large H_{ij} for large $|i-j|$) which produce sizable contributions to the eigenstates ("small components"). The account of those is, of course, beyond the BRM approach and they should rather be treated with the help of perturbation theory. These components play an important role in the problem of parity nonconservation in compound nuclei. A statistical approach to dealing with the small components was developed in [11].

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