Approach to energy eigenvalues and eigenfunctions from nonperturbative regions of eigenfunctions

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We study the approach to energy eigenvalues and eigenfunctions of Hamiltonian matrices with band structure from diagonalization of their truncated matrices. Making use of a generalization of Brillouin-Wigner perturbation theory, it is shown that in order to obtain approximate energy eigenvalues and eigenfunctions the sizes of truncated matrices should be larger than the nonperturbative regions of the eigenfunctions by several band width of the Hamiltonian matrix, with the nonperturbative regions being able to be estimated before the eigenfunctions are known. This prediction is checked numerically by the Wigner-band random-matrix model, which shows that 99% of eigenfunctions can be obtained when the sizes of truncated matrices are larger than those of the nonperturbative regions of the eigenfunctions by three band widths of the Hamiltonian matrix, on average.

Diagonalization of large-scale Hamiltonian matrices is of importance in a variety of physical fields, for example, in the shell-model approach to complex atoms and nuclei. Various methods have been developed in dealing with this problem in different cases (see, e.g., Refs. [1–4]). For models in which interaction couples independent particle basis states with finite distance only, the Hamiltonian matrices have band structure. For a Hamiltonian matrix of this kind, in order to obtain its eigenfunctions in a given energy region with a given accuracy, diagonalization of its truncated matrices with relatively small sizes would be enough (see, e.g., Refs. [5–7]). In practice, it was suggested that the sizes of truncated matrices be taken as $3\bar{\sigma}$ for the shell model [6], where $\bar{\sigma}$ is the mean value of the energy dispersion of basis states $|i\rangle$, $\sigma_i^2 = \langle i|(H-\langle i|H|i\rangle)^2|i\rangle = \Sigma_{j\neq i}|H_{ij}|^2$. In particular, for low-lying energy eigenvalues, exponential convergence has been found numerically with the increase of the sizes of truncated matrices [7].

It is known that eigenfunctions of Hamiltonian matrices with band structure are composed of two parts: central parts and tails with exponential or faster decay. Once the sizes of the central parts of the eigenfunctions can be estimated before diagonalization of the Hamiltonian matrices, estimation will also be possible for the sizes of the truncated matrices for obtaining approximate eigenfunctions. A possibility for the former estimation comes from a generalization of Brillouin-Wigner perturbation theory (GBWPT), which shows that each energy eigenfunction can be divided analytically into a perturbative (PT) part and a nonperturbative (NPT) part [8]. Recently, for the so-called Wigner-band random-matrix model [9], it was shown that central parts of eigenfunctions are on average composed of their NPT parts and the slope regions of their PT parts with the size of the bandwidth of the Hamiltonian matrix [11]. In this paper we will show that in the general case central parts of eigenfunctions should lie mainly in their NPT regions and a part of their PT regions, which can be estimated before the exact eigenenergies and eigenfunctions are known. As a result, NPT regions of eigenfunctions can be taken as starting points

for the sizes of the truncated matrices in the approach to the eigenfunctions. The effectiveness of this method will be studied numerically by the Wigner-band random-matrix model.

Consider a Hamiltonian of the form $H(\lambda)=H_0+\lambda V$, where H_0 is an unperturbed Hamiltonian for independent particles and λV represents a perturbation with a running parameter λ. The eigenstates of the Hamiltonians $H(\lambda)$ and H_0 will be denoted by $|\alpha\rangle$ and $|k\rangle$, respectively,

$$H(\lambda)|\alpha\rangle=E_\alpha(\lambda)|\alpha\rangle, \quad H_0|k\rangle=E_k^0|k\rangle, \qquad (1)$$

with the labels α and k in energy order. The unperturbed states $|k\rangle$ are taken as basis states in the Hilbert space. The matrix of $H(\lambda)$ in the H_0 representation has a band structure, i.e., the perturbation V does not couple remote basis states. In the GBWPT, an eigenstate $|\alpha\rangle$ is divided into two parts $|t_\alpha\rangle\equiv P_\alpha|\alpha\rangle$ and $|f_\alpha\rangle\equiv Q_\alpha|\alpha\rangle$ by two projection operators

$$P_\alpha=\sum_{|k\rangle\in S_\alpha}|k\rangle\langle k|, \quad Q_\alpha=\sum_{|k\rangle\in \bar{S}_\alpha}|k\rangle\langle k|=1-P_\alpha, \quad (2)$$

where S_α and $\bar{S}_\alpha$ are two sets of basis states with no overlap and including all the basis states in them. In Ref. [8], the operator P_α was defined by $P_\alpha=\Sigma_{k=p_1}^{p_2}|k\rangle\langle k|$ (the subscript α for p_1 and p_2 omitted). Here we extend it to the more general expression in Eq. (2). Following the arguments given in the appendix of Ref. [8], it is easy to show that $|f_\alpha\rangle$ can be expanded in a convergent perturbation expansion by making use of $|t_\alpha\rangle$ even when perturbation is strong,

$$|f_\alpha\rangle=T_\alpha|t_\alpha\rangle+T_\alpha^2|t_\alpha\rangle+\cdots+T_\alpha^n|t_\alpha\rangle+\cdots, \qquad (3)$$

if the sets S_α and $\bar{S}_\alpha$ are chosen to satisfy the condition

$$\lim_{n\to\infty}\langle\alpha|(T_\alpha^\dagger)^nT_\alpha^n|\alpha\rangle=0, \qquad (4)$$

where

$$T_\alpha = \frac{1}{E_\alpha - H^0} Q_\alpha \lambda V. \tag{5}$$

The part $|t_\alpha\rangle$ is said to be the NPT *part* and $|f_\alpha\rangle$ the PT *part* of $|\alpha\rangle$ in case that S_α has the smallest number of basis states and the expansion (3) is not truncated for each of the components of $|f_\alpha\rangle$ in the basis states $|j\rangle \in \bar{S}_\alpha$. Correspondingly, basis states in the set S_α and basis states in $\bar{S}_\alpha$ are termed the NPT *region* and the PT *region* of $|\alpha\rangle$, respectively.

A condition equivalent to Eq. (4) can be achieved by writing T_α^n in the form

$$T_\alpha^n = \frac{1}{E_\alpha - H^0} (\lambda U_\alpha)^{n-1} Q_\alpha \lambda V, \tag{6}$$

where

$$U_\alpha \equiv Q_\alpha V \frac{1}{E_\alpha - H^0} Q_\alpha \tag{7}$$

is an operator in the subspace spanned by basis states in $\bar{S}_\alpha$. Equation (6) shows that it is the properties of λU_α that determines whether $T_\alpha^n |\alpha\rangle$ vanishes when n goes to ∞. In fact, introducing eigenstates of the operator U_α, denoted as $|\nu_\alpha\rangle$, $U_\alpha |\nu_\alpha\rangle = u_{\alpha\nu} |\nu_\alpha\rangle$, the condition (4) is equivalent to the requirement that $|\lambda u_{\alpha\nu}| < 1$ for all $|\nu_\alpha\rangle$, if $\langle \nu_\alpha | Q_\alpha V | \alpha\rangle \neq 0$ for each $|\nu_\alpha\rangle$. The case that there exists a state $|\nu_\alpha\rangle$ for which $\langle \nu_\alpha | Q_\alpha V | \alpha\rangle = 0$, which is either quite rare or due to some symmetry of the Hamiltonian, is not to be discussed in this paper. Then, the condition (4) can be replaced by

$$\lim_{n \to \infty} \langle \phi | (T_\alpha^\dagger)^n T_\alpha^n | \phi\rangle = 0, \tag{8}$$

with $|\phi\rangle$ being an arbitrary state. When the eigenenergy E_α is not very close to any of the unperturbed energies E_k^0, the operator T_α is not sensitive to the value of E_α. Then, in order to give an estimation for the NPT region of a state in a given narrow energy region, one can use condition (8) with E_α replaced by an arbitrary value in the given energy region, that is, the estimation can be made before the exact eigenenergy and eigenfunction are known.

Expanding the state $Q_\alpha \lambda V |t_\alpha\rangle$ in the states $|\nu_\alpha\rangle$, $Q_\alpha \lambda V |t_\alpha\rangle = \Sigma_\nu h_\nu |\nu_\alpha\rangle$, and using the expansion of $|f_\alpha\rangle$ in Eq. (3), as in Ref. [11], one can show that the component of a perturbed state $|\alpha\rangle$ in a basis state $|j\rangle$ in its PT region, denoted by $C_{\alpha j} = \langle j | \alpha\rangle$, can be expressed as

$$C_{\alpha j} = \frac{1}{E_\alpha - E_j^0} \sum_\nu \left[\frac{h_\nu}{1 - \lambda u_{\alpha\nu}} \langle j | \nu_\alpha \rangle \right] (\lambda u_{\alpha\nu})^{m-1}, \tag{9}$$

where m is the smallest positive integer for $\langle j | T_\alpha^m | t_\alpha\rangle$, and equivalently $\langle j | (Q_\alpha V)^m | t_\alpha\rangle$ is not equal to zero. Such a state $|j\rangle$ is said to belong to the subregion A_α^m of the PT region of $|\alpha\rangle$, which by definition is the set of basis states $|k\rangle$ in the PT region satisfying $\langle k | (Q_\alpha V)^n | t_\alpha\rangle \neq 0$ with $n = 1, \ldots, m$. Since $|\lambda u_{\alpha\nu}| < 1$ for all $|\nu_\alpha\rangle$, each term on the right-hand

side of Eq. (9) decays exponentially with increasing m when m is larger than 1. Therefore, in general, central parts of eigenfunctions should lie mainly in their NPT regions and the subregions A_α^1 of their PT regions. These properties of eigenfunctions suggest that, in order to achieve good approximations to them, basis states for truncated matrices should include their NPT regions supplemented by basis states in some subregions A_α^m of their PT regions with not large m.

In the practical estimation of the NPT region of a state $|\alpha\rangle$, it is unnecessary to try all possible P_α and Q_α. In fact, since Eq. (8) is satisfied in case $|E_\alpha - E_k^0|$ are large enough for all the basis states $|k\rangle \in Q_\alpha$, one can use $P_\alpha = \Sigma_{k=p_1}^{p_2} |k\rangle\langle k|$ with $|k\rangle$ in increasing energy order and the corresponding Q_α to obtain a rough estimation for the NPT region. In practice, one can first take $p_1 = p_2 = \alpha$, then, increase p_2 and decrease p_1, until Eq. (8) is satisfied. Denoting the largest p_1 and smallest p_2 thus obtained, ensuring the validity of Eq. (8), as p_1^m and p_2^m, respectively, we have found numerically that the value of $\langle \phi | (T_\alpha^\dagger)^n T_\alpha^n | \phi\rangle$ increases quite fast with increasing n when the pair (p_1, p_2) is not close to (p_1^m, p_2^m). Therefore, the evaluation of p_1^m and p_2^m does not take much calculation time in practice. In order to obtain an approximation to the NPT region better than $\{|p_1^m\rangle, \ldots, |p_2^m\rangle\}$, one must take the detailed structure of the basis states into account, e.g., properties of the good quantum numbers in labeling the unperturbed states. For a quantum system with the underlying classical system being chaotic, one can expect that the difference between $\{|p_1^m\rangle, \ldots, |p_2^m\rangle\}$ and the exact NPT region of $|\alpha\rangle$ is not large and $\{|p_1^m\rangle, \ldots, |p_2^m\rangle\}$ can be taken as a practical estimation of the NPT region in the determination of the sizes of truncated matrices.

To test the above method of approaching the eigenfunctions numerically, we employ a simple model with band-structure Hamiltonian, namely, the Wigner-band random-matrix model (see, e.g., Refs. [10–13] for current interest). The Hamiltonian matrix of the model discussed in this paper is of the form

$$H_{ij} = (H^0 + \lambda V)_{ij} = E_i^0 \delta_{ij} + \lambda v_{ij}, \tag{10}$$

where $E_i^0 = i$ $(i = 1, \ldots, N)$ and off-diagonal matrix elements $v_{ij} = v_{ji}$ are random numbers with Gaussian distribution for $1 \leq |i - j| \leq b$ $(\langle v_{ij}\rangle = 0$ and $\langle v_{ij}^2\rangle = 1)$ and are zero otherwise. Here b is the bandwidth of the Hamiltonian matrix and N is its dimension. For this model, the projection operator P_α for the NPT region of a state $|\alpha\rangle$ is of the form $P_\alpha = \Sigma_{k=p_1}^{p_2} |k\rangle\langle k|$. The subregion A_α^m is composed of basis states $|k\rangle$ satisfying $p_1 - mb \leq k \leq p_1 - 1$ or $p_2 + 1 \leq k \leq p_2 + mb$. Central parts of the averaged eigenfunctions in the middle energy region of this model have been found lying in their NPT regions and the subregions A_α^1 (called the slope regions in Ref. [11]) of their PT regions.

Nonperturbative regions of low-lying eigenfunctions were not studied in Ref. [11]. Here we first show their features. In Fig. 1, we present the average shape of eigenfunctions,
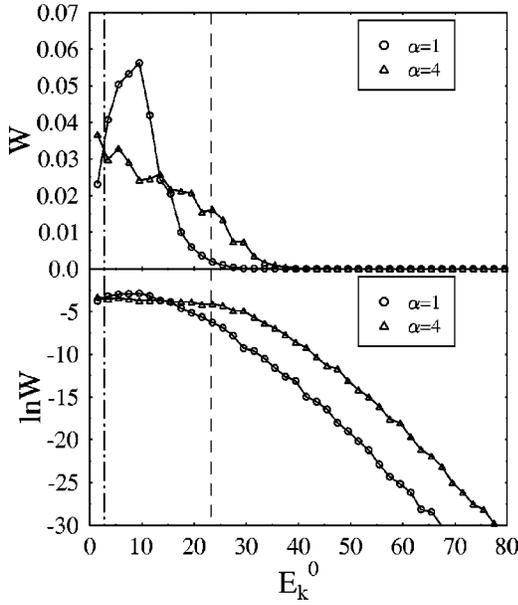
FIG. 1. The average shape $W=\langle C_{\alpha j}^2 \rangle$ of ground states ($\alpha=1$) (circles connected by solid curves) and of the third excited states ($\alpha=4$) (triangles connected by solid curves) for the Wigner-band random-matrix model with $\lambda=10$, $b=10$, and $N=500$. The vertical-dashed-dotted straight lines indicate the position of the average upper boundary $\langle p_2 \rangle$ of the NPT regions of the ground states and the vertical-dotted lines for the third excited states.

namely, $W=\langle C_{\alpha k}^2 \rangle$, for the ground state $\alpha=1$ and the third excited state $\alpha=4$ in the ordinary scale and logarithm scale, respectively, with the averaged upper boundaries of their NPT regions $\langle p_2 \rangle$. The average was taken over 50 realizations of the random matrices of the model with $N=500$, $b=10$, and $\lambda=10$. The lower boundaries of the NPT regions of the eigenfunctions are equal to one, $p_1=1$. We see that the main body of the average shape of the third excited states is composed of the averaged NPT part and the subregion A_α^1 of the averaged PT part. For the ground states, since the eigenenergies E_0 are much lower than E_4, the NPT regions are more narrow than those of $\alpha=4$ and the main body of their average shape extends to the subregion A_α^2 of the averaged PT part. Figure 2 shows the variation of $\langle p_2 \rangle$, $\langle p_1 \rangle$, and $\langle N_p \rangle = \langle p_2-p_1 \rangle$ with α when $\lambda=10$ and $b=10$. We see that in the low-energy region, the value of $\langle N_p \rangle$ is small, i.e., the NPT regions of the eigenfunctions are narrow. This is because eigenenergies in this energy region are either much smaller than or close to the lowest unperturbed energy E_1^0. The value of $\langle N_p \rangle$ becomes almost saturated when α is larger than 80. The values of $\langle p_2 \rangle$, $\langle p_1 \rangle$, and $\langle N_p \rangle = \langle p_2-p_1 \rangle$ in Fig. 2 were obtained by using condition (4) with exact eigenenergies and eigenstates. Approximations to them, as predicted above, can be obtained by making use of the condition (8) with E_α replaced by some values close to them (see, e.g., triangles in Fig. 2).

In studying the approach of results of truncated matrices to exact ones, it would be convenient to express the sizes of the truncated matrices with respect to the NPT regions of the exact eigenstates. Concretely, for a low-lying eigenfunction
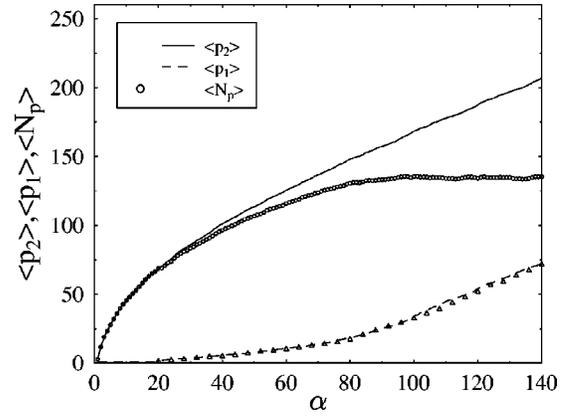

FIG. 2. The average boundary $\langle p_2 \rangle$, $\langle p_1 \rangle$, and the average size $\langle N_p \rangle = \langle p_2-p_1 \rangle$ of the NPT regions of eigenfunctions in the low-energy region. $N=500$, $b=10$, and $\lambda=10$. The triangles show part of the values for $\langle p_1 \rangle$ obtained from condition (8) with not exact values of E_α.

with $p_1=1$ and a truncated matrix taken in basis states $|k\rangle$ with $k=1,2,\ldots,k_t$, we use the value of $x=k_t-p_2$ to indicate the size of the truncated matrix. Denoting the eigenvalues and eigenstates in energy order of the truncated matrix as E_β^t and $|\beta^t\rangle$, respectively, the values of $\delta\psi_\alpha=1-|\langle \beta^t|\alpha\rangle|^2$ and $\delta E_\alpha=|E_\alpha-E_\beta^t|$ with $\beta^t=\alpha$ give measures for the approach of the results of the truncated matrix to the exact ones. When $p_1\neq1$, a truncated matrix is taken in basis states $|k_t^1\rangle$, $|k_t^1+1\rangle$, $\ldots$, $|k_t^2\rangle$ with $k_t^1=p_1-x$ and $k_t^2=p_2+x$ ($k_t^1=1$ if $x\geq p_1$). The value of δE_α is defined by the minimum of $|E_\alpha-E_\beta^t|$ and the value of $\delta\psi_\alpha$ is the corresponding value of $1-|\langle\beta^t|\alpha\rangle|^2$. Variation of the average values of $\delta\psi_\alpha$ and δE_α for α in different energy regions is shown in Fig. 3. We see that in both the low and the middle of the energy region the values of $\delta\psi$ decrease almost exponentially with increasing x when $x>20$. For δE, when $x>20$, the decay is even a little faster than exponential.
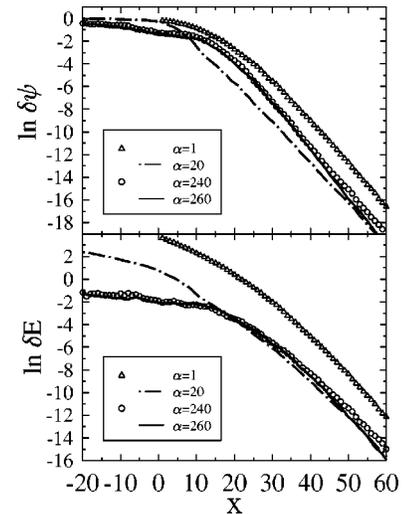

FIG. 3. Variations of the average values of δE_α and $\delta\psi_\alpha$ with x for $\alpha=1$ (triangles), 20 (dashed-dotted curve), 240 (circles), and 260 (solid curve) in logarithm scale ($\lambda=10, b=10$).
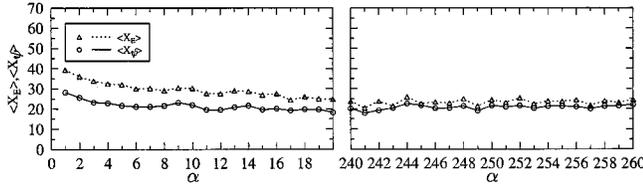
FIG. 4. The average values of X_E (triangles) and X_ψ (circles) for different states $|\alpha\rangle$.

We have studied the values of x at which $\delta E_\alpha(x) = 0.01$ and $\delta\psi_\alpha(x) = 0.01$, which will be denoted by X_E and X_ψ in what follows, respectively. The average values of X_E and X_ψ for states in the low ($\alpha = 1-20$) and the middle ($\alpha = 240-260$) of the energy region are given in Fig. 4. Both of them decrease when α changes from 1 to 20, which is in agreement with the behavior of eigenfunctions with respect to their NPT regions shown in Fig. 1. At $\alpha = 20$, the values of $\langle X_E \rangle$ and $\langle X_\psi \rangle$ are almost the same as those in the middle energy region, respectively. In both energy regions, $\langle X_E \rangle$ are larger than $\langle X_\psi \rangle$. The figure shows that in order to obtain 99% of eigenfunctions, truncated matrices larger than the NPT regions by $3b$ on each side would be enough on average. Note that, when $\lambda = 10$ and $b = 10$, $\langle N_p \rangle$ is less than 140, while $3\bar{\sigma} = 3000$. In this respect, the method discussed in this paper is more effective than the one making use of $\bar{\sigma}$ in giving the sizes of truncated matrices.

The results in Fig. 4 were obtained when $b = 10$ and $\lambda = 10$. For other values of the bandwidth b and the parameter λ, similar results have also been found. In Fig. 5 we present the variation of $\langle X_E \rangle/b$ with λ for $b = 5$, 10, and 20. The average was taken over the lowest 20 eigenstates ($\alpha = 1-20$) of 50 realizations of random Hamiltonian matrices. We see that the values of $\langle X_E \rangle/b$ are close to each other for different bandwidth b when λ is smaller than 4. In case of strong perturbation of $\lambda = 20$, the value of $\langle X_E \rangle/b$ is still less than 4 for $b = 20$. An interesting feature of $\langle X_E \rangle/b$ for $b = 5$ is that it decreases with λ when λ is larger than 6 (similar results also found for $b = 10$ and 20 when λ and N are large enough). This is due to the so-called localization of eigenfunctions in energy shell discovered in Ref. [12] and
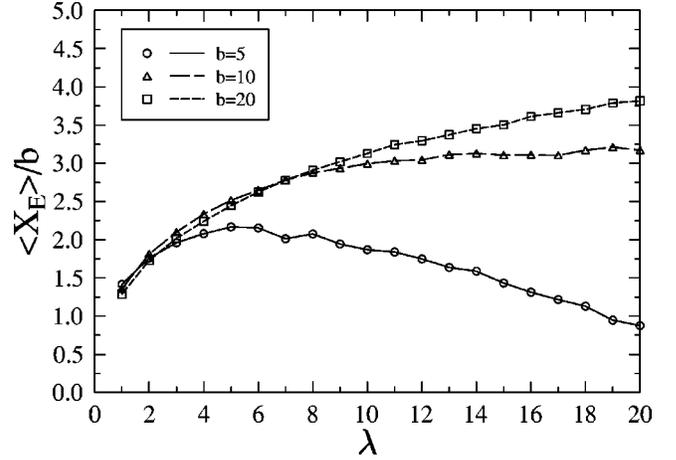

FIG. 5. Variations of $\langle X_E \rangle/b$ with λ for $b = 5$, 10, and 20.

explained in terms of properties of NPT parts of eigenfunctions in Ref. [11].

In conclusion, we have shown that the NPT regions of eigenfunctions, which can be estimated before the eigenfunctions are known, can be used as starting points in the approach to energy eigenvalues and eigenfunctions from diagonalization of truncated Hamiltonian matrices. For the Wigner-band random-matrix model, we have shown that, in order to obtain 99% of eigenfunctions, truncated matrices larger than the NPT regions by 3 bandwidth b of the Hamiltonian matrix would be enough on average when $b = 10$ and $\lambda = 10$. The sizes of truncated matrices given by this method have been found much smaller than $\bar{\sigma}$, the mean energy dispersion of basis states. This property would be useful in reducing the calculation time in obtaining approximate eigenfunctions. It is reasonable to expect that, not only for the Wigner-band random-matrix model but also for a variety of models of physical interest, the mean size of NPT regions be much smaller than $\bar{\sigma}$. In particular, for energy levels much lower than the lowest unperturbed energy, the NPT regions are usually quite small. Another feature of the method discussed in this paper is that the role of the bandwidth of the Hamiltonian matrix becomes quite clear in the determination of the accuracy of the method.

[1] S.E. Koonin, D.J. Dean, and K. Langanke, Phys. Rep. **278**, 1 (1997).
[2] H. De Raedt and M. Frick, Phys. Rep. **231**, 107 (1993).
[3] M. Honma, T. Mizusaki, and T. Otsuka, Phys. Rev. Lett. **77**, 3315 (1996).
[4] A. Novoselsky, M. Valliéres, and O. La'adan, Phys. Rev. Lett. **79**, 4341 (1997).
[5] O. Bohigas, S. Tomsovic, and D. Ullmo, Phys. Rep. **223**, 43 (1993).
[6] M. Horoi, B.A. Brown, and V. Zelevinsky, Phys. Rev. C **50**, R2274 (1994).
[7] M. Horoi, A. Volya, and V. Zelevinsky, Phys. Rev. Lett. **82**, 2064 (1999).
[8] Wen-ge Wang, F.M. Izrailev, and G. Casati, Phys. Rev. E **57**, 323 (1998).
[9] E. Wigner, Ann. Math. **62**, 548 (1955); **65**, 203 (1957).
[10] V.V. Flambaum, A.A. Gribakina, G.F. Gribakin, and M.G. Kozlov, Phys. Rev. A **50**, 267 (1994).
[11] Wen-ge Wang, Phys. Rev. E **61**, 952 (2000).
[12] G. Casati, B.V. Chirikov, I. Guarneri, and F.M. Izrailev, Phys. Lett. A **223**, 430 (1996).
[13] Y.V. Fyodorov, O.A. Chubykalo, F.M. Izrailev, and G. Casati, Phys. Rev. Lett. **76**, 1603 (1996).