Shifts of Random Energy Levels by a Local Perturbation

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We consider the effect of a local perturbation on the energy levels of a system described by random matrix theory. An analytic expression for the joint distribution function of initial and final energy levels is obtained. In the case of unitary ensemble we also find the two-point correlation function of initial and final densities of states. [S0031-9007(97)05246-0]

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The random matrix theory [1-3] of energy levels in complex systems was developed in the 1950s for the description of the absorption spectra of large nuclei. In this approach one gives up any attempt to study the position of each particular resonance, but instead concentrates on the characteristics averaged over a large number of resonances. The positions of the resonances are identified with the eigenvalues of some matrix, and the averaging is performed over the elements of this matrix.

The statistical properties of the eigenvalues ε_i of a Hermitian random matrix \hat{H} of size $N \times N$ are completely described by their joint distribution function $P(\{\varepsilon_i\})$, which can be written in the following simplified form:

$$P(\{\varepsilon_i\}) \propto \prod_{i>j} (\varepsilon_i - \varepsilon_j)^{\beta}.$$
 (1)

Here the energies ε_i are ordered: $\varepsilon_i < \varepsilon_{i+1}$; the exponent $\beta = 1, 2, 4$ for ensembles of orthogonal, unitary, and symplectic matrices, respectively.

Expression (1) vanishes when any two energy levels approach each other; this effect is commonly referred to as *level repulsion*. This repulsion can also be illustrated by rewriting $P({\varepsilon_i})$ as

$$P(\{\varepsilon_i\}) = e^{-\beta E}, \qquad E = -\sum_{i>j} \ln(\varepsilon_i - \varepsilon_j).$$
 (2)

Thus $P(\{\varepsilon_i\})$ can be interpreted as Gibbs distribution of a gas of classical particles at points ε_i with logarithmic repulsion between them. In physically interesting situations there must be a finite average distance Δ between the particles (energy levels). This is usually achieved by either introducing a parabolic confining potential $\delta E = \alpha \sum_i \varepsilon_i^2$ or by confining the particles to a circle [4].

More recently the random matrix theory was applied to a number of physically different systems, such as metallic grains [5,6] and microwave cavities [7]. In these systems one can easily modify the matrix \hat{H} , e.g., by applying magnetic field to the grain or by deforming the microwave cavity. Such modification can be described by a perturbation \hat{V} , and one is usually interested in the correlations of the energy levels of the old and new systems described by matrices \hat{H} and $\hat{H} + \hat{V}$. Dyson [8] suggested to describe such correlations in terms of the viscous Brownian motion of the infinitely heavy particles (2) with the same logarithmic interactions between them. The external perturbation in this approach plays the role of the fictitious time in which the Brownian motion occurs. What remains then is to find the distribution of the positions of all the particles after some time t, provided initial distribution (1). Time t can be related to the characteristic value of the potential \hat{V} , so that the parametric correlations are universal functions of only one parameter.

However, the Brownian-motion approach is not always applicable. Consider a perturbation of the general form

$$\hat{V} = N \sum_{i=1}^{N} v_i |i\rangle \langle i|, \qquad (3)$$

where $|i\rangle$ form a complete set of states, and the matrix dimension N is included for proper definition of limit $N \rightarrow \infty$. For the Brownian-motion model to be applicable [8,9], the condition $v_i \ll \Delta$ must hold, where Δ is the mean level spacing. Since $N \gg 1$, the sum $\sum_i v_i^2$ which has the meaning of the fictitious time t in the Brownian-motion picture, can still be arbitrarily large.

In a number of interesting physical situations one deals with a local perturbation described by Eq. (3) with $v_i = v \delta_{i1}$, where v is not necessarily small. An example of such perturbation is a short-range impurity in a metallic grain. When such an impurity is added to the system, its levels ε_i shift to new positions λ_i . The new many-particle ground state $|\Psi\rangle$ has a rather small overlap with the old one, $|\Phi\rangle$; this phenomenon [10] is called orthogonality catastrophe. The overlap can be expressed in terms of the old and new energy levels:

$$|\langle \Psi | \Phi \rangle|^2 = \prod_{i=1}^{M} \prod_{j=M+1}^{N} \frac{(\lambda_j - \varepsilon_i) (\varepsilon_j - \lambda_i)}{(\lambda_j - \lambda_i) (\varepsilon_j - \varepsilon_i)}, \quad (4)$$

where *M* is the number of electrons in the system [11]. Therefore to treat the orthogonality catastrophe in a metallic grain one needs the knowledge of the joint distribution function $P(\{\varepsilon_i\}, \{\lambda_i\})$ of *both* old and new energy levels.

The determination of this joint distribution function is the main subject of this paper. The Brownian-motion model is not applicable in this case, but a closed analytic expression for $P(\{\varepsilon_i\}, \{\lambda_i\})$ can be found directly. For the orthogonal, $\beta = 1$, and unitary, $\beta = 2$, ensembles we will show that

$$P(\{\varepsilon_i\},\{\lambda_i\}) \propto \frac{\prod_{i>j} (\varepsilon_i - \varepsilon_j) (\lambda_i - \lambda_j)}{\prod_{i,j} |\varepsilon_i - \lambda_j|^{1 - \beta/2}} \times \exp\left[-\frac{\beta}{2\nu} \sum_i (\lambda_i - \varepsilon_i)\right].$$
(5)

Energy levels in Eq. (5) are constrained by the condition

$$\begin{aligned} \varepsilon_i &\leq \lambda_i \leq \varepsilon_{i+1}, & \text{if } v > 0, \\ \varepsilon_{i-1} &\leq \lambda_i \leq \varepsilon_i, & \text{if } v < 0. \end{aligned}$$
(6)

Equation (5) is the central result of this paper.

To derive Eq. (5) we need to relate the eigenvalues λ_j of the perturbed matrix $\hat{H} + \nu N |\nu\rangle \langle \nu|$ to the unperturbed eigenvalues ε_i and eigenfunctions $|i\rangle$; here $|\nu\rangle$ is an arbitrary vector. This is easily accomplished:

$$\sum_{i} \frac{A_{i}}{\lambda_{j} - \varepsilon_{i}} = \frac{1}{\nu N}, \qquad A_{i} \equiv |\langle \nu | i \rangle|^{2}.$$
(7)

Equation (7) enables one to find $P(\{\varepsilon_i\}, \{\lambda_i\})$ given the joint distribution function of unperturbed eigenvalues and eigenfunctions. Since the distributions of eigenvalues and eigenvectors in the random matrix theory are uncorrelated, we have

$$P(\{\varepsilon_i\},\{\lambda_i\}) = P(\{\varepsilon_i\})p(\{A_i\}) \left| \det\left[\frac{\partial A_i}{\partial \lambda_j}\right] \right| .$$
(8)

Here $P(\{\varepsilon_i\})$ is the distribution function (1) of the unperturbed energy levels, and $p(\{A_k\})$ is the eigenvector distribution function, which at $N \to \infty$ is given by the Porter-Thomas [13] formula:

$$p(\lbrace A_i \rbrace) = \prod_i \frac{N}{(2\pi N A_i)^{1-\beta/2}} \exp\left(-\frac{\beta}{2} N A_i\right), \quad (9)$$

where $\beta = 1$ or 2. Finally, the last factor in Eq. (8) is the Jacobian of the transformation from the eigenvector variables A_i to the new energies λ_i .

To find the distribution function (8) we do not need to solve Eq. (7) with respect to λ_j . In order to find the Jacobian in Eq. (8) one only has to solve (7) with respect to A_i . The latter is a much simpler problem since Eq. (7) is linear in A_i , and the solution can be expressed in terms of Cauchy determinants. This readily yields

$$A_{i} = \frac{1}{\nu N} \frac{\prod_{j=1}^{N} (\lambda_{j} - \varepsilon_{i})}{\prod_{j \neq i} (\varepsilon_{j} - \varepsilon_{i})}.$$
 (10)

By definition all A_i are positive; see Eq. (7). This immediately gives constraint (6). It follows from Eq. (10) that

$$\frac{\partial A_i}{\partial \lambda_j} = \frac{A_i}{\lambda_j - \varepsilon_i} \,. \tag{11}$$

As a result of the Jacobian in Eq. (8) is reduced to a Cauchy determinant, and we obtain

$$\det\left[\frac{\partial A_i}{\partial \lambda_j}\right] = \frac{1}{(N\upsilon)^N} \frac{\prod_{j>i} (\lambda_j - \lambda_i)}{\prod_{j>i} (\varepsilon_j - \varepsilon_i)}.$$
 (12)

In order to express the Porter-Thomas distribution function (9) in terms of the energies ε_i and λ_j we need to evaluate the sum $\sum_i A_i$. To this end we sum up both sides of identity (11) over *i*, and using Eq. (7), find

$$\frac{\partial}{\partial \lambda_j} \sum_i A_i = \frac{1}{N \upsilon}, \qquad j = 1, \dots, N.$$

We therefore conclude that the sum of A_i is a linear function of all λ_i is a linear function of all λ_i . The constant can be determined by noticing that according to Eq. (10) at $\lambda_i \rightarrow \varepsilon_i$ we have $A_i \rightarrow 0$. Thus

$$\sum_{i} A_{i} = \frac{1}{Nv} \sum_{i} (\lambda_{i} - \varepsilon_{i}).$$
(13)

Finally, we substitute Eqs. (1), (9), and (12) into Eq. (8), and with the help of Eqs. (10) and (13) get the joint distribution function Eq. (5). Strictly speaking, the result (5) is valid only in the limit $N \rightarrow \infty$. This is the physically most interesting regime where the properties of the system are universal.

If one is interested in nonuniversal corrections associated with the finite size of the matrix, the Porter-Thomas distributions (9) should be replaced by [4]

$$p(\{A_i\}) = \frac{\Gamma(\beta N/2)}{\Gamma(\beta/2)^N} \left(\prod_i A_i\right)^{\beta/2-1} \qquad \delta\left(1 - \sum_i A_i\right).$$
(14)

As a result, the exponential factor in Eq. (5) is replaced [14] by $\delta(1 - (N\nu)^{-1}\sum_i (\lambda_i - \varepsilon_i))$. However, for practical calculations the distribution function in the form (5) is more convenient.

Our result (5) contains complete information about distribution of the old and new energy levels of the system. In applications, such as analysis of experimental spectra, one often needs only a small part of this information, which is contained in *n*-level correlation functions. The most important of them is the two-point correlation function of the old and new densities of states K_2 . We define this quantity as

$$K_2(s) = \frac{1}{\rho^2(E)} \times \sum_{ik} \left\langle \delta \left(E + \frac{s}{2} - \lambda_i \right) \delta \left(E - \frac{s}{2} - \varepsilon_k \right) \right\rangle.$$

 $K_2(s)$ has the meaning of the probability to find a new level at a distance *s* from a given old level. The correlation function K_2 does not depend on energy *E*, provided that *s* is much smaller than the characteristic energy scale over which average density of states $\rho(E) =$ $\sum_i \langle \delta(E - \lambda_i) \rangle$ varies.

We have been able to obtain a compact analytic expression for $K_2(s)$ for the unitary ensemble only, and we outline the derivation below. Because K_2 does not

depend on the particular shape of $\rho(E)$, it is convenient to get rid of energy dependence of $\rho(E)$ by adopting the circular ensemble of Dyson [2], where all *N* levels are put on the circle of unit radius. Equation (5) for $\beta = 2$ then takes the form

$$P_{c} = \left[\prod_{i>j} 4 \sin\left(\frac{\varepsilon_{i} - \varepsilon_{j}}{2}\right) \sin\left(\frac{\lambda_{i} - \lambda_{j}}{2}\right)\right] \times e^{-\frac{1}{\nu}\sum_{i}(\lambda_{i} - \varepsilon_{i})}.$$
(15)

Here the energies are measured in dimensionless units and defined within the interval $[-\pi, \pi]$; we have also omitted the normalization constant. Mean level spacing in such a model is given by $\Delta = 2\pi/N$.

We express function K_2 in terms of the functional derivative

$$K_{2} = \frac{\Delta^{2}}{I[\mathcal{A}, \mathcal{B}]} \frac{\delta^{2} I[\mathcal{A}, \mathcal{B}]}{\delta \mathcal{A} \delta \mathcal{B}} \bigg|_{\mathcal{A}, \mathcal{B}=0}$$
(16a)

of the generating functional for v > 0 (negative v are considered analogously)

$$I = \int_{-\pi}^{\pi} d\varepsilon_1 \int_{\varepsilon_1}^{\pi} d\lambda_1 \int_{\lambda_1}^{\pi} d\varepsilon_2 \int_{\varepsilon_2}^{\pi} d\lambda_2 \dots \int_{\lambda_N}^{\pi} d\lambda_N P_c$$
$$\times \prod_k [1 + \mathcal{A}(\varepsilon_k)] [1 + \mathcal{B}(\lambda_k)]. \tag{16b}$$

Following the procedure similar to that of Ref. [2], we find that the generating functional I can be rewritten as a determinant of a certain matrix $I = \det \hat{F}$, where

$$F_{kl} = \int_{-\pi}^{\pi} d\varepsilon \int_{\varepsilon}^{\pi} d\lambda e^{(v^{-1}+ik)\varepsilon - (v^{-1}+il)\lambda} \times [1 + \mathcal{A}(\varepsilon)][1 + \mathcal{B}(\lambda)].$$
(17)

We then expand the determinant up to the second order in small sources \mathcal{A} and \mathcal{B} . This expansion requires the knowledge of the matrix \hat{F}^{-1} at $\mathcal{A} = \mathcal{B} = 0$, which in the limit $N \to \infty$ takes the form $F_{kl}^{-1} = \delta_{kl} \frac{v^{-1} + ik}{2\pi}$. Substituting the result in Eq. (16a) we obtain after simple algebra [15]

$$K_{2} = 1 - \left[\theta(r) - \int_{-\infty}^{r} dr' e^{\frac{r'\Delta}{\nu}} \frac{\sin \pi r'}{\pi r'}\right] \\ \times \frac{\partial}{\partial r} \left[e^{-\frac{r\Delta}{\nu}} \frac{\sin \pi r}{\pi r} \right], \qquad (18)$$

where $r = s/\Delta$ is the energy in the units of the level spacing. The result (18) is valid for positive *v*; for v < 0 one should substitute $r \rightarrow -r$ in Eq. (18).

Let us now discuss asymptotic behavior of the twopoint correlation function (18). In the limit of vanishing perturbation $v \rightarrow 0$, we immediately obtain $K_2 = \delta(r) + 1 - (\sin \pi r / \pi r)^2$ which is the well-known result for the two-point correlation function of the unitary ensemble [3,4]. In the limit $r \gg 1$, ν/Δ , the integration in Eq. (18) can be easily performed and we find

$$K_2 = 1 - \frac{\sin^2(\pi r - \delta)}{(\pi r)^2},$$
 (19)

where $\delta = \arctan(\pi v / \Delta)$ is the phase shift of the scattering off of the impurity. The sequence of periodic maxima of the correlation function (19) is a signature of the level repulsion, and the average shift δ of the new levels with respect to the old ones is consistent with the Friedel sum rule $\langle \lambda_i - \varepsilon_i \rangle / \Delta = \delta / \pi$.

In conclusion, we studied the statistics of shifts of eigenvalues of a random Hamiltonian by a local perturbation of arbitrary strength. Despite the fact that the conventional Brownian motion model is not applicable, we have found the whole joint distribution function of old and new levels, Eq. (5), and the correlator of the old and new densities of states (18). Using Eq. (4), these results can be applied to the study of orthogonality catastrophe in small metallic grains.

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