New Approach to the Statistical Properties of Energy Levels

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The joint distribution of energy eigenvalues of a Hamiltonian is derived by means of the usual statistical laws of classical many-body systems. It makes a transition from the Poisson type to the Gaussian type depending on the value of a single parameter characteristic of the Hamiltonian.

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The random-matrix theories have been the most powerful tool for the study of the excitation spectra of heavy nuclei in the neutron-capture region.[1,2] Among others the Gaussian orthogonal ensemble (GOE) has given the best account of fluctuation phenomena of neutron resonance levels in nuclei. Although comparisons are still limited, the atomic- and the molecular-level fluctuations also fit the GOE prediction significantly.[3] Despite the different natures of interaction, either strong short range or electromagnetic long range, they indicate the universality of level fluctuations in complex bound systems. The remarkable success of the random-matrix theory naturally raises the questions: What is the origin of the randomness? What is the origin of the universality of level fluctuations? Recently numerical calculations of the quantal spectra of two-dimensional Hamiltonian systems have paid much attention to the exploration of the quantum-mechanical manifestation of classical chaotic motion in level fluctuations. There are some numerical evidences that the fluctuation patterns show a transition from the Poisson type to the GOE type as the corresponding classical system shifts from the integrable to the chaotic regime.[4,5] It raises another question: How do the specific features of the Hamiltonian influence the patterns of fluctuations?

In this paper I wish to answer these fundamental questions by making use of the laws of ordinary statistical mechanics instead of introducing *a priori* ensembles of random matrices. The important attempt toward the resolution of the problem was initiated by Pechukas[6] who studied the motion of energy spectra in the semiclassical limit as $\hbar$ varies to zero. Here, I shall consider the motion of levels for a system defined by the Hamiltonian

$$H = H_0 + tV,$$

as the perturbation strength t increases. The eigenvalues $\{x_n(t)\}$ are assumed to be discrete and nondegenerate except for accidental degeneracies. The eigenfunctions $\{\phi_n(t)\}$ are real orthonormal and form a complete set. The equations of motion for $x_n(t)$ and the various matrix elements $V_{mn}(t) = \langle \phi_m(t) | V \times | \phi_n(t) \rangle$ can be obtained from the stationary Schrödinger equation together with the completeness condition in the same manner as in Ref. 6. By the trivial changes of variables

$$p_n = V_{nn}, \quad f_{mn} = |x_m - x_n| V_{mn} \quad (n \neq m),$$

one gets without any approximation

$$dx_n/dt = p_n, \tag{1}$$

$$\frac{dp_n}{dt} = 2 \sum_{m(\neq n)} \frac{f_{nm}^2}{(x_n - x_m)^3}, \tag{2}$$

$$\frac{df_{nm}}{dt} = (x_n - x_m) \sum_{l(\neq n,m)} \frac{f_{nl} f_{lm}}{|x_n - x_l||x_l - x_m|} \left(\frac{1}{x_n - x_l} + \frac{1}{x_m - x_l} \right) \quad (x_n > x_m). \tag{3}$$

There exist infinite numbers of integrals of the motion. The simplest ones are $A_{a0} = \mathrm{Tr} V^a$ ($a = 1, 2, 3, \ldots$). In general, when the quantity $\mathrm{Tr}G$ does not contain t explicitly, it is a constant of the motion because of the representation independence of trace. They can be written as $A_{ab} = \mathrm{Tr}G_{ab}$ for the operator G_{ab} constructed by a linear superposition of the polynomial $V^a H^b$ and all the possible combinations obtained from it by permutations of V and H in such a manner that the explicit t dependence vanishes; for example,

$$A_{22} = \mathrm{Tr}[V^2 H^2 - (VH)^2],$$

$$A_{32} = \mathrm{Tr}[V^3 H^2 - V(VH)^2],$$

etc.

Imagine the motion of N particles (i.e., N sequences of levels) in a "box" of size L and take the coordinate frame such that the box is at rest.[7] Under these conditions the quantities A_{ab} with $a = 1$ or $a \geq 3$ are not integrals of the motion any more, since they contain terms involving odd powers in p_n. The only remaining integrals of the motion

$$A_{2b} = \sum_{\mu=0}^{b} C_\mu \mathrm{Tr}(VH^\mu VH^{b-\mu}) \tag{4}$$

can be determined by taking the coefficients C_μ so

that the explicit t-dependent terms cancel:

$$0=\partial A_{2b}/\partial t$$
$$=2\sum_{\mu}C_{\mu}\sum_{\nu}\mathrm{Tr}(VH^{\nu}VH^{\mu-\nu-1}VH^{b-\mu}). \quad (5)$$

In Eq. (4) the number of free parameters C_μ grows linearly as b increases, while the number of independent terms in Eq. (5), i.e.,

$$\mathrm{Tr}(VH^{n_1}VH^{n_2}VH^{n_3})$$

with $n_1+n_2+n_3=b-1$, increases quadratically with b. Thus it will soon become impossible to achieve the complete cancellation of t-dependent terms by any choice of C_μ as b gets larger, and it is enough to consider first several quantities A_{2b}. In fact, only A_{20} and A_{22} turn out to be integrals of the motion of the TrG type. They are written as

$$E=\tfrac{1}{2}A_{20}=\tfrac{1}{2}\sum_{n}P_n^2+\tfrac{1}{2}\sum_{n\neq m}\frac{f_{nm}^2}{(x_n-x_m)^2}, \quad (6)$$

$$Q=\tfrac{1}{2}A_{22}=\tfrac{1}{2}\sum_{n\neq m}f_{nm}^2. \quad (7)$$

It is interesting to notice that the canonical equations of motion regarding Eq. (6) as the Hamiltonian coincide with Eqs. (1) and (2).

It is now clear that the system we are considering is quite analogous to the classical dynamical system of N particles in one dimension confined in a box of size L and interacting mutually through the time-dependent $1/r^2$ potential. Let us now turn to the statistical properties of this system. The phase space has the dimensionality of $2N+\frac{1}{2}[N(N-1)]$ composed of the dynamical variables $\{x_n\}$, $\{p_n\}$, and $\{f_{nm}\}$. We denote them all together as $\{y_i\}$. According to the method of statistical mechanics we introduce the ensemble of subsystems[8] distributed in phase space with a probability

$$dw=\rho(\{y_i\},t)\prod_i dy_i.$$

After a sufficiently long interval of time the system will be in a state of statistical equilibrium.[9] The continuity equation for steady flow gives

$$\sum_i\frac{\partial(\rho\dot{y}_i)}{\partial y_i}=0.$$

According to the equations of motion the velocities $\{\dot{y}_i\}$ are not functions of y_i itself. Thus we have Liouville's theorem

$$d\rho/dt=\sum_i(\partial\rho/\partial y_i)\dot{y}_i=0,$$

which says that the distribution function must be expressible entirely in terms of the integrals of the motion. We have constructed two integrals of the motion E and Q which are additive. Since it is known[10] that in a finite-dimensional space all the invariants under orthogonal transformation can be expressed in the form TrG, there should be no other integrals of the motion. Thus the stationary distribution function of the subsystems is given by

$$\rho=\frac{1}{Z}\exp(-\beta E-\gamma Q), \quad (8)$$

with

$$Z=\int e^{-\beta E-\gamma Q}\prod_i dy_i.$$

The parameters β and γ are determined by given values of the conserved quantities E_0 and Q_0 through the relationships

$$E_0=-\frac{\partial\ln Z}{\partial\beta},\quad Q_0=-\frac{\partial\ln Z}{\partial\gamma}.$$

As far as level distributions are concerned, the integrations over the unobserved variables $\{P_n\}$ and $\{f_{nm}\}$ may be carried out, which gives

$$P(\{x_n\})\prod_n dx_n$$
$$=C_N\sum_{m>n}\left[\frac{(x_m-x_n)^2}{1+(\gamma/\beta)(x_m-x_n)^2}\right]^{1/2}\prod_n dx_n, \quad (9)$$

with the normalization constant

$$c_N^{-1}=\frac{1}{N!}\int_0^L\int dx_n\cdots dx_1\prod_{m>n}\left[\frac{(x_m-x_n)^2}{1+(\gamma/\beta)(x_m-x_n)^2}\right]^{1/2}.$$

The parameter γ/β links the statistical nature of energy eigenvalues to the Hamiltonian of a particular system. Now, I shall show important consequences of the distribution at extreme limits of the parameter: For the study of the case of small γ/β, Eq. (9) may be written as

$$P(\{x_n\})\propto\exp\left[-\sum_{m>n}A_{mn}\right],$$

with

$$A_{mn}=-\ln|x_m-x_n|+\tfrac{1}{2}\ln[1+(\gamma/\beta)(x_m-x_n)^2].$$

If we approximate the second term as

$$\ln[1+(\gamma/\beta)(x_m-x_n)^2]\simeq(\gamma/\beta)(x_m-x_n)^2,$$

the level distribution reads

$$P(\{x_n\})\propto\exp\left[\sum_{m>n}\ln|x_m-x_n|-\frac{N\gamma}{2\beta}\sum_n(x_n-x_0)^2\right]. \quad (10)$$

This looks exactly like the distribution of the GOE ex-

cept for one point: $x_0 = N^{-1}\sum_n x_n$ is the center-of-mass coordinate here, whereas it is an external parameter in the GOE. Equation (10) can give a natural account of the average level density also. In the GOE it is given by the semicircle distribution due to the Gaussian factor with a fixed center x_0. On the other hand, the translation-invariant form (10) implies a constant average density N/L in the box of size L. Thus we can avoid the difficulty of the GOE in reproducing the average property of levels by approximating the level density stepwise with the density N_i/L_i for the ith energy interval L_i.

In the opposite limit $\gamma/\beta \to \infty$, $P(\{x_n\})$ is approximately constant except near degeneracies $x_n \simeq x_m$. This distribution is known as the Poisson distribution. The nearest-neighbor spacing distribution in this case can be easily calculated, which gives

$$P_0(S) \sim \frac{(L-S)^{N-1}/(N-1)!}{L^N/N!},$$

which reduces to $\rho e^{-\rho S}$ in the "thermodynamical" limit $N, L \to \infty$ with N/L finite $(=\rho)$. For values of the parameter γ/β between these two limits we expect that the nearest-neighbor spacing will have a form similar to the Brody distribution,[11] i.e.,

$$P_0(S) \sim S^{\nu} \exp(-aS^{\nu+1}),$$

since Eq. (9) exhibits level repulsion at any value of γ/β.

Without introducing *a priori* ensembles of random matrices we have derived the level distribution function by making use of the ensemble in the ordinary statistical mechanics, i.e., the ensemble of subsystems. The relation to the random-matrix theory can be understood formally by writing the distribution function in terms of the original variables $\{x_n\}$ and $\{V_{mn}\}$:

$$dw \sim \exp(-\beta E - \gamma Q) \prod_{m>n} |x_m - x_n| \prod_n dx_n \prod_{m \geq n} dV_{mn},$$

where $\prod_{m>n} |x_m - x_n|$ is the Jacobian. By integration over $\{x_n\}$ it reads

$$dp \sim \exp(-\tfrac{1}{2}\beta \operatorname{Tr} V^2) D(V) \prod_{m \geq n} dV_{mn},$$

with

$$D(V) = \int \exp\left(-\gamma \sum_{m>n} (x_m - x_n)^2 V_{mn}^2\right) \prod_{m>n} |x_m - x_n| \prod_n dx_n.$$

This can be interpreted as the distribution of the ensemble of random perturbation matrices $\{V_{mn}\}$, where $D(V)$ takes into account correlations between the matrix elements. When $\gamma = 0$, the correlation disappears (i.e., $D = \text{const}$) and the distribution reduces to the GOE type for $\{V_{mn}\}$.

In obtaining the distribution (9) I have assumed the laws of the ordinal statistical mechanics, namely, the system reaches equilibrium after a long enough time interval with a canonical distribution for the ensemble of subsystems. However, the relaxation time should not be too long since we wish to keep the density of states constant during the relaxation period. In order to check its validity I have made numerical integrations of the equations of motion by truncating interactions f_{mn} after the next-nearest levels (i.e., $f_{mn} = 0$ for $|m-n| \geq 3$). The nearest-neighbor spacing distributions tend to converge to stationary distributions after reasonable time intervals with the typical relaxation time $\tau_x \lesssim 1$, while the relaxation of velocities to the Maxwell distribution is quite slow $(\tau_p > 1)$. This is because of the one-dimensional nature of the system where the energy-momentum conservation law does not allow the change of momenta in binary collisions. Faster relaxation of velocity can be expected when we include more interactions beyond next-nearest ones. Details of the numerical results will be reported elsewhere.

We have limited our discussion to stationary distributions. In principle, there will exist transitional distributions when a system does not relax to equilibrium in a reasonable interval of time.[12] For example, we can imagine a system close to integrable so that the specific nature of the unperturbed Hamiltonian H_0 remains in the level distribution for a long time interval. Thus, there could be a great variety of fluctuation patterns in nature. However, the universality of the GOE suggests that most of the Hamiltonians of complex bound systems such as nuclei, molecules, and atoms have small values of γ/β. It will be desirable to calculate the parameters β and γ for various Hamiltonians to understand the universality. Also, the calculation in two-dimensional Hamiltonian systems will give us important information about the relation between classical chaos and the quantal spectra.

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