Distribution of energy levels of quantum systems

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It is suggested that the distribution of the spacings between adjacent energy levels of quantum systems be described as an uncorrelated superposition of a Landau-Wigner-Dyson distribution for the irregular parts of the spectrum and a Poisson distribution for the regular part.

1. We consider a quantum-mechanical system with a discrete spectrum. We construct a distribution function in the spacing between adjacent energy levels, $p(t)$, by working from the condition that $p(\rho S)\rho dS$, where ρ is the level density in the given part of the spectrum, is that fraction of the levels for which the distance to the neighboring level lies in the interval between S and $S + dS$. This function was first intro-

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duced to describe the highly excited states of heavy nuclei (see Ref. 1 and the bibliography cited there). It is now used widely in a variety of problems, even if there are only a few degrees of freedom. This function has attracted interest because its behavior is intimately related to the problem of the semiclassical quantization of nonintegrable systems.[2,3] The distribution function is known with physical rigor in two limiting cases:

$$p(t) \approx \begin{cases} \exp(-t) & \text{for classical integrable systems,} \quad (1a) \\ \frac{\pi}{2} t \exp\left(-\frac{\pi}{4} t^2\right) & \text{for ergodic systems.} \quad (1b) \end{cases}$$

Most systems, however, do not conform to either of these cases. A simple example of such a system is that with the Hamiltonian

$$H = \frac{1}{2}(p_1^2 + q_1^2) + \frac{1}{2}(p_2^2 + q_2^2) + 4kq_1^2 q_2^2 , \quad (2)$$

which describes massive Yang-Mills fields that depend on a single variable.[4] Haller *et al.*[5] have numerically calculated the energy levels for this system and have constructed a histogram of the distribution of spacings between adjacent levels in various parts of the spectrum for various values of the coupling constant k. It turns out that all the distributions can be approximated well by the function

$$p_q(t) = (1+q)\beta t^q \exp(-\beta t^{1+q}), \qquad \beta = \{\Gamma((2+q)/(1+q))\}^{1+q} , \quad (3)$$

which had been proposed earlier for fitting the distributions of adjacent levels of heavy nuclei.[1] The parameter q turns out to be a smooth function of the classical parameter kE. In the present letter we construct a distribution function for systems of this type, working from the properties of the classical phase space.

2. We know that for typical Hamiltonian systems with $N \geqslant 2$ degrees of freedom the phase space can be partitioned into sets of two types, organized in a complicated way[2,3,6,7]:

a) a regular set consisting of points lying on invariant tori, as for integrable systems;

b) an irregular set, in which all the trajectories are unstable, so that the behavior of the typical trajectories, almost all of which are ergodic on the $(2N-1)$-dimensional set, is very complicated (or even stochastic).

With each such set, which has a phase volume $\gtrsim h^N$, where h is Planck's constant, we associate a system of semiclassical levels, whose number in the given part of the spectrum is proportional to the phase volume of this set. With the regular set we associate a system of regular levels, little different from the levels of integrable systems. In particular, it can be shown that the overlap integral of two regular wave functions, which appears in the expression for the repulsion of two levels with approximately equal energies, is small, and the distribution function is of the form in (1a). In turn, we associate with the irregular region a system of irregular levels, for which the overlap integral is large, and $p(t)$ is approximately the same as (1b). Since the different sets are assumed to be nonintersecting, the overlap integral of the levels from different

regions is small, and these levels do not experience any significant repulsion. In a study of the overlap integral, it is convenient to use the formalism of Wigner functions,[2] which, in the semiclassical approximation, are nonzero only near the region of ergodicity of a typical classical trajectory, according to Ref. 2.

3. The high-lying energy levels of quantum systems can thus be partitioned into groups associated with the regular and irregular sets in the phase space. In the i-th group, the probability for a neighboring level of the same group to lie between S and $S + dS$ is known, equal to $p_i(\rho_i S)\rho_i dS$, where ρ_i is the density of levels of the given group, and $p_i(t)$ is the distribution function. For regular levels, $p_i(t)$ is given by (1a), while for irregular levels it is given by (1b). The resultant distribution of any neighboring levels is found as an uncorrelated superposition of the distribution functions of all the groups.

4. To determine this distribution, we construct the following functions for each group of levels, using the procedure of Ref. 8:

$$F_i(t) = \int_0^t p_i(y)dy\,, \qquad E_i(t) = \int_t^\infty (1 - F_i(y))dy\,. \tag{4}$$

The function $F_i(t)$ is the probability that the distance between the levels of the i-th group is $\leqslant t$, while $E_i(t)$ is the probability that an interval of length t will be free of levels of the i-th group. Knowing $E_i(t)$ for all the groups, we construct the two new functions

$$E(t) = \prod_i E_i(f_i t)\,, \qquad p(t) = \frac{d^2E(t)}{dt^2}\,, \tag{5}$$

where $f_i = \rho_i/\rho$ and $\rho = \Sigma_i \rho_i$ is the total density of all levels ($\Sigma_i f_i = 1$). It follows from the independence of the levels of different groups that $E(t)$ is the probability that the interval of length t will be free of levels of all groups, while $p(t)$ is the distribution function of all adjacent levels, which we are seeking.

5. The quantity f_i in (5) is the relative density of levels in the i-th group. In the semiclassical approximation it is equal to the fraction of the phase volume of the given part of the spectrum which is occupied by the i-th set of trajectories and depends on only the parameters of the classical problem; the discrete symmetry of the problem is taken into account. The number of factors in (5) is equal to the number of nonintersecting regular and irregular sets. It can be shown, however, that the ultimate result depends on the total volume occupied by the invariant tori and is independent of the complicated structure of the regular set. For systems with two degrees of freedom, there is an infinite number of irregular regions with decreasing phase volume.[6,7] Two circumstances limit the growth of the number of regions: 1) For quantum-mechanical problems, regions with a volume less than h^N may be ignored. 2) If there exist n irregular regions, for which we have $f_i \to 0$, but for which $\Sigma_i f_i$ is bounded, then the distribution function of the corresponding levels tends toward (1a) in the limit $n \to \infty$. For systems with $N > 2$ degrees of freedom, there is apparently only a single irregular region in all cases.[6,7]

We thus see that $E(t)$ in (5) contains a single factor with distribution function (1a), which corresponds to a regular set and to small irregular sets, and one or several

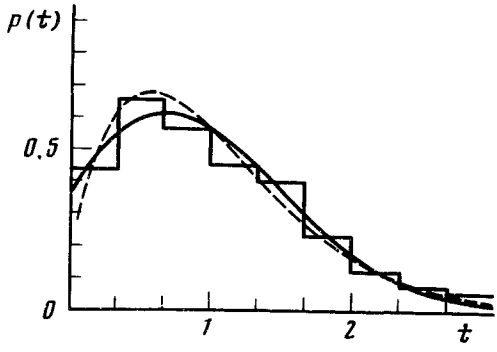

FIG. 1. Distribution of the spacings between neighboring, completely symmetric levels for system (2) with $k = 0.005$ and $85 < E < 135$. Histogram—Numerical distribution of 469 levels found in Ref. 5; dashed curve—approximating distribution (3) with $q = 0.548$ from Ref. 5; solid curve—distribution (6) with the calculated value $f_I(0.55) \approx 0.8$.

factors corresponding to large irregular sets, for which $p_i(t)$ is given by (1b). Here is the explicit expression for distribution function (5) for the particular case of one irregular region:

$$p(t) = \left(y\left(\frac{\sqrt{\pi}}{2} f_I t\right) f_R^2 + \frac{\pi}{2} t f_I^3 + 2 f_I f_R \right) \exp\left(- f_R t - \frac{\pi}{4} f_I^2 t^2 \right), \tag{6}$$

where $y(z) = 2/\sqrt{\pi} \exp(z^2) \int_z^\infty \exp(-t^2) dt$, f_I is the fraction of the phase volume of the given part of the spectrum which is occupied by the irregular region (the symmetry of the problem is taken into account), and $f_R = 1 - f_I$.

Expression (6) is the basic result of this study.

6. Let us compare (6) with function (3), which is frequently used to fit the experimental distributions of neighboring levels.[1,5] For all $0 \leqslant q \leqslant 1$ we can choose $f_I(q)$ in such a way that the difference between the functions (6) and (3) is small everywhere except in a small vicinity of $t = 0$ (Fig. 1). At the prevailing accuracy, one distribution function cannot reliably be distinguished from the other. Figure 2 shows f_I as a function of kE for model (2), found from the kE dependence of q (see Fig. 2b in Ref. 5). Also shown in this figure are several values of f_I found through a direct numerical calculation of the fraction of the phase volume occupied by the irregular region. To determine this quantity, we partitioned the constant-energy surface into small cells and calculated the number of cells through which a typical irregular trajectory passes

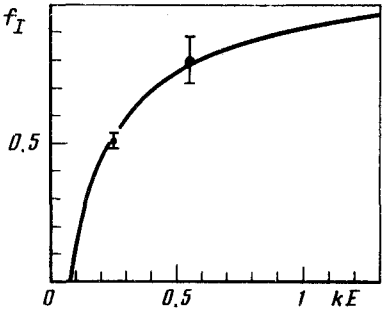

FIG. 2. The fraction of the phase volume occupied by the irregular region as a function of the parameter kE for system (2). Curve—The result of a conversion of the function $q(kE)$ from Ref. 5; points—results of direct calculations.

over a long time. The error bars shown in this figure reflect the boundedness of the number of partitions and of the computation time; the errors could be reduced substantially by carrying out more lengthy calculations.

7. In conclusion we wish to emphasize that although the assumptions on which the derivation of distribution function (6) is based are rather crude, this distribution function has a clear physical meaning, and it approximates the results of Ref. 5 as well as approximating distribution (3) does. An important property of distribution (6) is that for simple systems like (2) it allows an independent calculation for which it is sufficient to find the phase volumes occupied by the different irregular sets.

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