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Distribution of degeneracies in simple quantum systems

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Abstract. In some simple quantum mechanical systems, the degeneracy of typical energy levels grows as a power of the energy or size. We ask whether, after dividing out this average growth, there is a well defined probability distribution of scaled degeneracies in the limit of large size or energy. The answer is yes, for a free particle in a sphere or cube. For the sphere, the distribution of scaled degeneracies is shown to follow a circular law. For the cube, a numerical study shows that the distribution rises linearly for low values of the scaled degeneracy and decays exponentially for large values.

Keywords. Energy spectrum; degeneracies; statistical properties.

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1. Introduction

The statistical properties of the spectra of simple quantum-mechanical systems have been studied extensively in recent years. One of the principal objects of study has been the probability distribution of spacings between successive energy levels. This spacing distribution varies from random-matrix like, for quantum analogues of classically chaotic systems (Berry 1983), to Poissonian, for generic integrable systems like a particle in a cuboid with irrational aspect ratios (Shudo 1989), to a finite series of delta functions, as for rational cuboids (Subrahmanyam and Barma 1990).

The principal point of this paper is to define and study a different characteristic of the eigenvalue spectrum—namely the distribution of degeneracies. The degeneracy of a typical individual level may or may not grow with the energy or size, and if it does, the reason may or may not be related to a symmetry. For example, the degeneracy of energy levels is strictly bounded for a free particle in an irrational cuboid. But for a free particle in a sphere or rational cuboid, typical degeneracies grow without bound as the energy increases; in the former instance, large degeneracies are a consequence of an obvious symmetry, and in the latter case not.

We are interested in systems with growing degeneracies, and the characterization of the degeneracy distribution. Consider an energy interval $(e, e+\Delta e)$, where Δe is small compared to e, but large enough to contain many levels (throughout this paper, we use 'level' to denote the location of an energy eigenvalue; each level corresponds to many eigenstates). The mean value of the degeneracy (on averaging over all levels in the range Δe) typically grows as a power of e. For the sphere and cube, as we shall see later, the mean degeneracy grows as $e^{1/2}$, and so we are led to examine a scaled degeneracy $d \equiv \text{degeneracy}/e^{1/2}$ for both these systems. Figure 1 shows a plot of d versus $e^{1/2}$, for both sphere and cube. The conventional energy spacing distribution

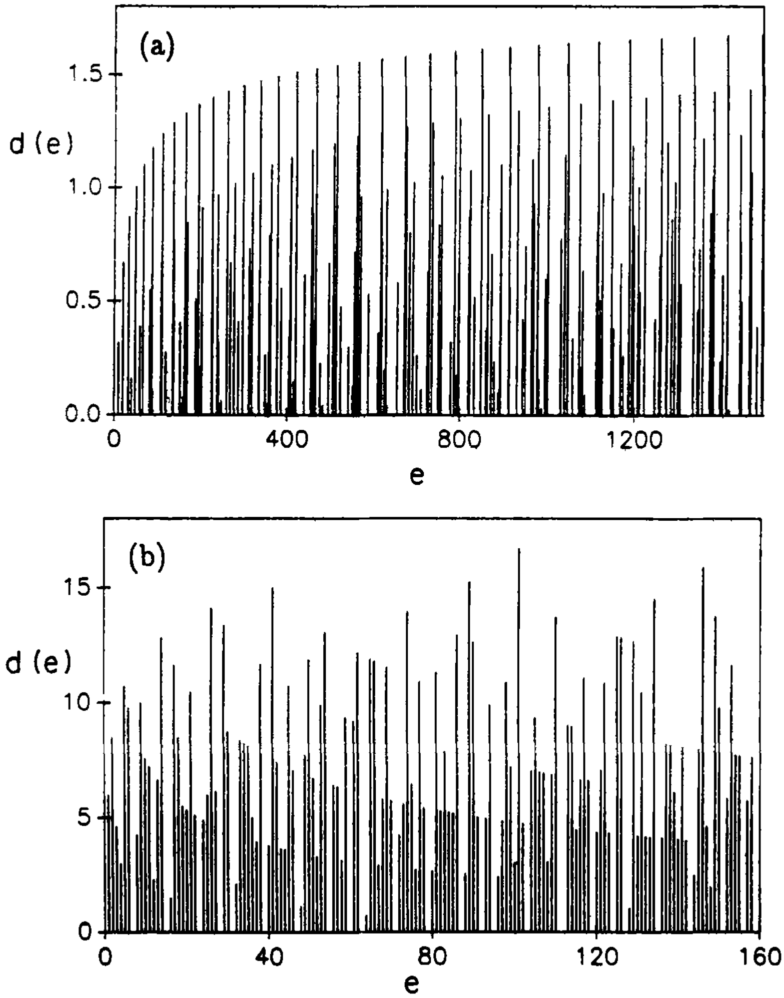

Figure 1. The scaled degeneracy $d(e) \equiv (\text{degeneracy})/e^{1/2}$ plotted against the scaled energy e for a particle in (a) a sphere with Dirichlet boundary conditions (b) a cube with periodic boundary conditions.

characterizes the distribution of gaps in the locations along the abscissa, while the degeneracy distribution that is of interest here describes the fluctuations of heights along the ordinate. Of all the levels with energy in the range $(e, e + \Delta e)$, let $f(d, e)\Delta d$ be the fraction which have a value of scaled degeneracy in the range $(d, d + \Delta d)$. The questions we would like to answer are: In the limit $e \to \infty$, is there a limiting distribution

$$P(d) \equiv \lim_{e \to \infty} f(d, e) \tag{1}$$

which describes degeneracy probabilities? If so, what is its form?

The mean degeneracy of levels in a square billiard system has been estimated (Berry 1981), and the root mean square degeneracy in a general system has been related to the mean degeneracy of classical periodic orbits (Biswas *et al* 1991). But, to our knowledge, the existence and the form of the full distribution $P(d)$ have not been investigated earlier.

For the sphere, where degeneracies are specified in terms of a single quantum number, it is possible to find $P(d)$ in closed form (§ 2). For the cube, the value of the mean scaled degeneracy is found analytically, but not the full distribution of degeneracies; both the existence and form of $P(d)$ are established numerically (§ 3) in this case.

2. Degeneracy distribution for a sphere

Consider a free particle of mass m inside a hard-walled sphere of radius R. Eigenstates are labelled by the principal, orbital and azimuthal quantum numbers n, l, M respectively, and the energy eigenvalues are given by

$$\varepsilon_{nl} = \frac{\hbar^2}{2mR^2}\alpha_{nl}^2 \tag{2}$$

where α_{nl} denotes the location of the nth zero of the lth order spherical Bessel function. That ε does not depend on the azimuthal quantum number M reflects the spherical symmetry of the system, and results in a $(2l+1)$-fold degeneracy for a level with orbital angular momentum l. We define a dimensionless energy $e \equiv 2mR^2\varepsilon/\hbar^2$, and the scaled degeneracy as

$$d \equiv \frac{2l+1}{e^{1/2}}. \tag{3}$$

In order to find the degeneracy distribution $P(d)$ for large e, one can use the Debye approximation for larger order Bessel functions (Abramowitz and Stegun 1965). Within this approximation, the nth zero of the lth order spherical Bessel function is located at $e \equiv k^2$, with

$$\begin{aligned} l + 1/2 &= k\cos\phi \\ (n - 1/4)\pi &= k(\sin\phi - \phi\cos\phi) \end{aligned} \tag{4}$$

where ϕ varies between 0 and $\pi/2$.

Consider an energy interval corresponding to the interval $(k, k+\Delta k)$. The number of levels (with different (n, l)) which lie in this range, and also in the l-range $(l, l+\Delta l)$, is then $(\partial n/\partial k)_l \Delta k\, \Delta l$. Using (4), the partial derivative can be evaluated to yield $\sin\phi/\pi$. Using (3) and (4) and normalizing, the probability distribution function, $P(d)$ is found to be

$$P(d) = \frac{4}{\pi}(1 - d^2/4)^{1/2}. \tag{5}$$

The degeneracy distribution is thus characterized by a circular law. Two qualitative aspects of the distribution should be noted. First, there is a strict cut-off, and no weight for arbitrarily large d. Second, the probability density is largest at $d = 0$. As we shall see below, the distribution is quite different from that for the cube, in both these respects.

3. Degeneracy distribution for a cube

Consider a particle inside a cube of edge length L, with periodic boundary conditions. Energy eigenvalues are then

$$\varepsilon_{n_x n_y n_z} = \frac{(2\pi\hbar)^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2) \tag{6}$$

where each of n_x, n_y and n_z runs over all integers. The possibility of large degeneracies arises from the different ways of writing an integer as the sum of three squares.

Gauss proved that an integer cannot be written as the sum of three squares if and only if it can be written as $4^l(8t + 7)$, where l and t are non-negative integers (Sierpinski 1964). Knowing this, it is possible to deduce the probability distribution of spacings (i.e. gaps in the spectrum) between energy levels. The result is a series of three delta functions, with known weights (Subrahmanyam and Barma 1990).

One can also deduce the mean degeneracy of an energy level as follows. From Gauss's results it follows that a fraction $\frac{1}{8}(1 + \frac{1}{4} + \frac{1}{4^2} + \cdots) = \frac{1}{6}$ of all integers cannot be written as the sum of three squares. If we define the scaled energy $e \equiv mL^2\varepsilon/2(\pi\hbar)^2$, the mean degeneracy $\bar{D}(e)$ must satisfy

$$\frac{5}{6}\bar{D}(e)\Delta e = 2\pi e^{1/2}\Delta e \tag{7}$$

where the right hand side is the number of states between e and $e + \Delta e$, and 5/6 on the left hand side is the number-theoretic factor reflecting the fraction of integers that actually correspond to energy eigenvalues.

From (7) we see that the mean degeneracy grows as $e^{1/2}$. Thus we define the scaled degeneracy $d(e) = \text{degeneracy}/e^{1/2}$. We did a numerical study to determine the distribution $P(d)$ of scaled degeneracies. Figure 2 shows the distribution of degeneracies determined from the first N levels of the spectrum, with $N = 8{\cdot}2 \times 10^3$ and 525×10^3. The results point to the existence of a limiting distribution as N increases indefinitely.

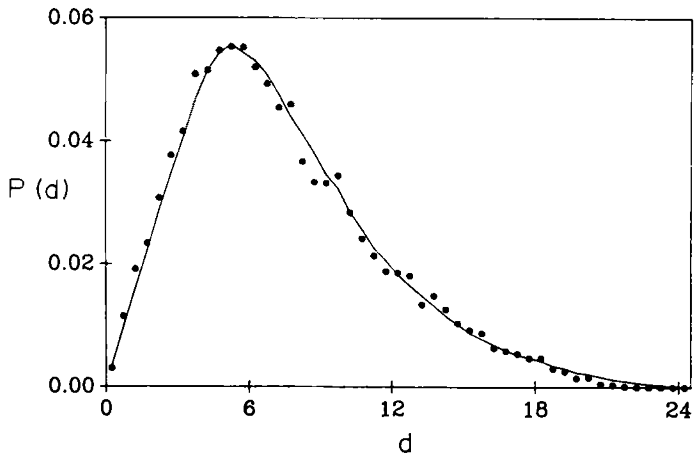

Figure 2. The degeneracy distribution for a cube, determined from the first N levels, with $N = 8{\cdot}2 \times 10^3$ (dots) and $N = 525 \times 10^3$ (continuous line).

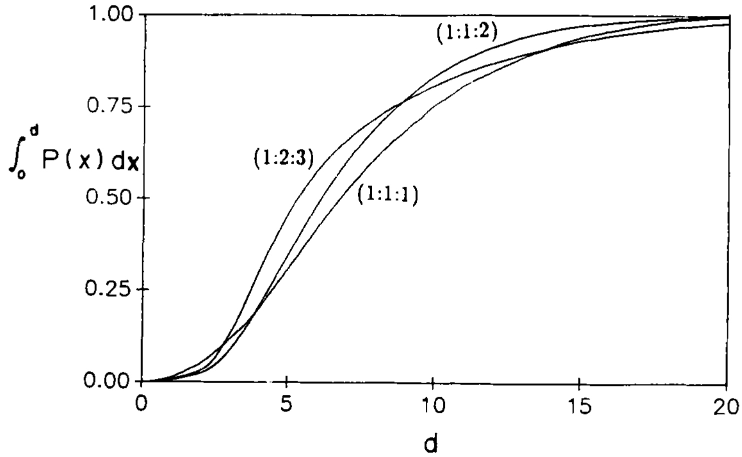

Figure 3. The integral of the degeneracy distribution for cuboids with squares of the sides in the ratios 1:1:1, 1:1:2 and 1:2:3. The distributions are not identical, but have broadly similar features.

The fact that the distributions shown in the figure have a cut-off at large d is related to the finiteness of N; the cut-off advances to infinity as N increases. The numerically determined distribution is well fit to a linear form $P(d) \sim d/d_0$ for low d, with $d_0 \simeq 0{\cdot}013$. At large d, the limiting distribution decays exponentially $\sim \exp(-d/d_\infty)$ with $d_\infty \simeq 7{\cdot}54$. We have not been able to fit the distribution to any known or very simple form.

Since degeneracies in a cube have a number-theoretic origin, it is interesting to ask whether other related systems also display similar systematics. To this end, we investigated cuboids with the squares of the sides in the ratio of simple integers 1:1:2 and 1:2:3. In figure 3 we show results for the cumulative probabilities $\int_0^d dx\, P(x)$ for the cube and the two cuboids. As can be seen from the figure, the distributions are not identical, but have broadly similar features: $P(d)$ grows linearly with d for low d, and decays exponentially for large d.

4. Conclusion

In systems where the degeneracies of levels grow as the size is increased, we can ask whether the (scaled) degeneracies are described by a well-defined probability distribution.

The answer is yes, for a free particle in a sphere and in a cube. In the former case, the distribution is described by a quarter circle law (eq. 5). In the latter case, numerical study establishes the form of the distribution (figure 2), which varies linearly for small d and falls exponentially for large d. The distributions for the cuboids studied are different in detail, but not in broad features, from that of the cube.

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Note added in proof

After this paper was submitted for publication, we came to know of a related study of the probability distribution of degeneracies for the cube (C Itzykson and J M Luck 1986 *J. Phys.* **A19** 211). We thank Prof. Itzykson for bringing this reference to our attention.