Level clustering in the regular spectrum

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In the regular spectrum of an f-dimensional system each energy level can be labelled with f quantum numbers originating in f constants of the classical motion. Levels with very different quantum numbers can have similar energies. We study the classical limit of the distribution P(S) of spacings between adjacent levels, using a scaling transformation to remove the irrelevant effects of the varying local mean level density. For generic regular systems $P(S) = e^{-S}$, characteristic of a Poisson process with levels distributed at random. But for systems of harmonic oscillators, which possess the non-generic property that the 'energy contours' in action space are flat, P(S) does not exist if the oscillator frequencies are commensurable, and is peaked about a non-zero value of S if the frequencies are incommensurable, indicating some regularity in the level distribution; the precise form of P(S) depends on the arithmetic nature of the irrational frequency ratios. Numerical experiments on simple two-dimensional systems support these theoretical conclusions.

1. Introduction

Percival (1973) has conjectured that there are two kinds of spectrum for a bound system which is almost classical and which has more than one degree of freedom. The regular spectrum occurs when the classical motion is integrable, that is there exists as many constants of motion as the number f of degrees of freedom; then each energy level is labelled by f quantum numbers $\{m_1 \dots m_f\} \equiv m$. The irregular spectrum occurs when there do not exist f constants of motion (e.g. in an ergodic system where only the energy is conserved); it is then impossible to label levels by f quantum numbers. It would be possible to distinguish the two sorts of levels by their different behaviour under perturbation, i.e. by their matrix elements.

The work reported here began with the thought that a simpler characterization of the difference between the regular and irregular spectra might be obtained by studying the probability distribution P(S) of the spacing S between adjacent levels. The argument proceeds by analogy with the 'statistical theory of spectra' (Porter 1965), where the level structure of complex nuclei and atoms (in which f is large

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and which are far from being classical) is modelled by the eigenvalue structure of random matrices. If the levels are uncorrelated, P(S) will simply be the negative exponential characteristic of Poisson processes such as radioactive decay, whose maximum value occurs at S=0, indicating strong level clustering. This behaviour is indeed found experimentally if level sequences with different values of fundamental quantum numbers (total angular momentum and parity) are superposed. If, however, the levels with given values of these quantum numbers are considered in isolation, strong correlations are observed, in the form of 'repulsion' between adjacent levels (i.e. P(0)=0); this repulsion occurs also for eigenvalues of random matrices.

On this basis it seemed possible that the levels of the irregular spectrum might repel one another, and that the levels of the regular spectrum might be uncorrelated. The first possibility has not been investigated. This paper is concerned with the second, that is, with a study of level spacing distributions for the regular spectrum. The astonishing result emerges that for the simplest regular systems, which are f-dimensional harmonic oscillators, the levels are correlated and the correlation consists of a repulsion between adjacent levels. Moreover, the behaviour of the spacings depends on the arithmetic nature of the frequency ratios of the oscillators, i.e. on whether these ratios are rational or irrational and, if irrational, whether the irrationalities are algebraic or transcendental. For all other classically integrable systems the levels are not correlated; this was expected but hard to prove. This theory is confirmed by numerical experiments on two-dimensional systems involving up to 10 000 levels, presented in §§ 4 and 6. Casual readers should concentrate on these results, and skip the theory in §§ 3 and 5.

The regular spectrum is perfectly deterministic: for each set of quantum numbers m the energy level E_m can be obtained from an explicit formula (equation 2.1). Probability distributions arise in the classical limit as Planck's constant \hbar vanishes and the number of levels in any range of energy increases limitlessly.

2. SCALING THE LEVELS

In an integrable classical system the constants of motion can be combined into f 'actions' $\mathbf{I} = \{I_1 \dots I_f\}$ which can be the new momenta in a canonical transformation from the original coordinates and momenta. The transformed Hamiltonian H depends only on \mathbf{I} . In terms of $H(\mathbf{I})$, the level m in the regular spectrum has energy

$$E_{m} = H(\mathbf{I} = (m + \frac{1}{4}\alpha)\hbar). \tag{2.1}$$

The vector α consists of f integers related to caustics of the classical trajectories with actions \mathbf{I} ; for the matters discussed here, α is irrelevant and will be set equal to zero (this corresponds to a shift in the origin of \mathbf{I} space). The result (2.1) is a semi-classical approximation which was obtained (with increasing sophistication and rigour) by Einstein (1917), Brillouin (1926), Keller (1958) and Maslov (1972); a careful discussion of its meaning and application is given by Percival (1976).

For the systems studied here (oscillators, particles in boxes, and combinations of these) all components of **I** are non-negative, so that only the positive 'quadrant' (really 2^f ant) in **I** space is physically meaningful. According to (2.1) this 'quadrant' is quantized into a 'square' lattice whose unit cells have side \hbar . As E increases from zero (taken as corresponding to $\mathbf{I} = 0$), the 'energy contour' $H(\mathbf{I}) = E$ expands into **I** space from its origin. Levels occur whenever this contour crosses a lattice point. We wish to study the statistics of such crossings.

Now E is an unsuitable parameter to describe the levels, for two reasons. The first is that the *mean level density* $\overline{n}(E)$ depends on energy. In fact $\overline{n}(E)$ is given by the 'Thomas–Fermi' formula

 $\overline{n}(E) = (1/h^f) d$ (phase space 'volume' for which H < E)/dE

$$= (1/\hbar^f) \int_{\substack{\text{positive} \\ \text{`quadrant'}}} d^f I \delta(E - H(\mathbf{I}))$$
 (2.2)

(for derivations see, for example, Berry & Mount 1972; Berry & Tabor 1976). The second reason is that the statistics of the levels might themselves depend on the region of energy being studied.

The simplest solution to this problem (and one that emphasizes its semi-classical nature) is to work at fixed E, and think of (2.1) as quantizing \hbar to values \hbar_m implicitly defined by

$$E = H(mh_m). (2.3)$$

(This amounts to thinking of a level m as a trajectory in the E, \hbar plane, and finding where this trajectory intersects a line with fixed E, instead of the customary fixed \hbar). However, the density of levels in \hbar is still non-uniform, and we scale \hbar by defining a new variable U as the total number of states below energy E for given \hbar ; from (2.2) this is

$$U \equiv (1/\hbar^f) \int_{\substack{\text{positive} \\ \text{ouadrant'}}} d^f I \Theta(H(\mathbf{I}) - E), \tag{2.4}$$

where Θ is the unit step function. The scaled levels U(m) are obtained by solving (2.3) for \hbar_m and substituting the value thus found into (2.4). The scaled level density is defined as

$$\rho(U) \equiv \sum_{m} \delta(U - U(m)). \tag{2.5}$$

The sum here is over all integer lattice points in and on the boundary of the positive 'quadrant' in m space; however U(m) is also defined through equations (2.3) and (2.4) as a continuous function of m.

The following equivalent properties follow from the definition of $U(\mathbf{m})$: First, the mean level density $\bar{\rho}(U)$ is unity, which was one of the purposes behind the scaling. This implies that the 'area' of the positive quadrant of \mathbf{m} space cut off by the contour $U(\mathbf{m}) = U_0$ is U_0 itself, i.e.

$$\int d^f m \Theta(U_0 - U(\boldsymbol{m})) = U_0. \tag{2.6}$$

Secondly, U(m) is a homogeneous function of m of degree f, i.e.

$$U(\beta \mathbf{m}) = \beta^f U(\mathbf{m}). \tag{2.7}$$

Therefore the form of any contour U(m) = U is obtained from the contour U(m) = 1 by expanding each radius vector by $U^{1/f}$. As U increases, the contours expand into m space from its origin, crossing lattice points at unit mean rate; we wish to study the statistics of these crossings as $U \to \infty$ (which from (2.4) corresponds to the semi-classical limit $\hbar \to 0$).

The action Hamiltonian $H(\mathbf{I})$ determines U(m) but the converse is not true since the homogeneous functions (2.7) form a smaller set than the possible Hamiltonians – in plain terms the introduction of U(m) normalizes away the information contained in $H(\mathbf{I})$ about the mean level spacing. Here are some specific forms for U(m) that will be employed later:

Case I. Harmonic oscillator with frequencies $\omega = \{\omega_1 \dots \omega_f\}$. The Hamiltonian is

$$H^{\mathbf{I}}(\mathbf{I}) = \boldsymbol{\omega} \cdot \mathbf{I} \tag{2.8}$$

and

$$U^{I}(\mathbf{m}) = \frac{(\boldsymbol{\omega} \cdot \mathbf{m})^{f}}{f! \prod_{i=1}^{f} \omega_{i}}.$$
 (2.9)

Case II. Particle of mass μ in f-dimensional box with sides $\{a_1 \dots a_f\}$. The Hamiltonian is

$$H^{\text{II}}(\mathbf{I}) = \pi^2 / 2\mu \sum_{i=1}^f I_i^2 / a_i^2$$
 (2.10)

and

$$U^{II}(\mathbf{m}) = \frac{(\frac{1}{4}\pi)^{\frac{1}{2}f} \prod_{i=1}^{f} a_i}{\Gamma(1 + \frac{1}{2}f)} \left[\sum_{i=1}^{f} \frac{m_i^2}{a_i^2} \right]^{\frac{1}{2}f}.$$
 (2.11)

Case III. Particle in a two-dimensional potential well with hard walls in one direction and harmonic binding in the other. The Hamiltonian is

$$H^{\text{III}}(\mathbf{I}) = \alpha I_1 + \beta I_2^2 \tag{2.12}$$

and

$$U^{\rm III}(\boldsymbol{m}) = \frac{1}{3} (4E_{\beta}/\alpha^2)^{\frac{3}{2}} m_2^4 [(m_1^2 + (4E_{\beta}/\alpha^2) m_2^2)^{\frac{1}{2}} - m_1]^{-2}. \tag{2.13}$$

Case IV. Perturbed two-dimensional oscillator. The Hamiltonian is

$$H^{\rm IV}({\bf I}) = (\omega_1 I_1 + \omega_2 I_2)^2 + \epsilon I_1^2 \tag{2.14}$$

and

$$U^{\text{IV}}(\boldsymbol{m}) = \frac{\left[(\omega_1 m_1 + \omega_2 m_2)^2 + \epsilon m_1^2 \right]}{2\omega_2 e^{\frac{1}{2}}} \arcsin\left(\left\lceil \frac{\epsilon}{\omega_1^2 + \epsilon} \right\rceil^{\frac{1}{2}} \right). \tag{2.15}$$

(As
$$\epsilon \to 0$$
, $U^{\text{IV}}(\boldsymbol{m}) \to U^{\text{I}}(\boldsymbol{m})$ with $f = 2$.)

From these examples the peculiar property of the harmonic oscillator (case I) is clear: only for this system are the contours of U(m) flat—they are hyperplanes in m space (equation 2.9). This will turn out to be of crucial importance. In the generic case the contours U(m) = constant are curved, and we restrict ourselves here to cases where these contours are convex away from m = 0, as in cases II—IV if all parameters are positive.

3. THE GENERIC CASE: THEORY

It is not convenient to study the scaled level density in the form (2.5); for large U the contours of U(m) are large and lattice points m may cross at widely separated points, and it is not obvious how these crossings are correlated (intuition suggests that they are not correlated—this turns out to be true generically but false for oscillators). To get a more transparent form, $\rho(U)$ is first transformed by the Poisson sum formula into a series of integrals over the positive 'quadrant' of m space:

$$\rho(U) = \sum_{\boldsymbol{m}} \int d^{f} m \delta(U - U(\boldsymbol{m})) e^{2\pi i \boldsymbol{M} \cdot \boldsymbol{m}}.$$
 (3.1)

M is an f dimensional lattice of positive and negative integers. The term M = 0 is the mean scaled level density, namely unity, and the terms $M \neq 0$ give the fluctuations $\Delta \rho(U)$ in which we are interested. The scaling law (2.7) gives

$$\Delta \rho(U) \equiv \rho(U) - 1 = \sum_{M=0} \int d\boldsymbol{m} \delta(1 - U(\boldsymbol{m})) \exp(2\pi i \boldsymbol{M} \cdot \boldsymbol{m} U^{1/f})$$

$$\equiv \sum_{M=0} \rho_{\boldsymbol{M}}(U).$$
(3.2)

The delta function confines the m integrals to the contour U(m) = 1, which will henceforth be called \mathscr{C} . With the use of f-1 curvilinear coordinates $\mu = \{\mu_1 \dots \mu_{f-1}\}$ on \mathscr{C} (figure 1), the 'partial fluctuations' ρ_M become

$$\rho_{\mathbf{M}}(U) = \int_{\mathscr{C}} \mathrm{d}^{f-1} \mu \frac{\exp\left(2\pi \mathrm{i} \mathbf{M} \cdot \mathbf{m}(\mu) \ U^{1/f}\right)}{|\nabla U(\mathbf{m}(\mu))|}.$$
 (3.4)

For large U (semi-classical case), the integrand oscillates rapidly as μ changes, and the dominant contributions come from points $\mu = \mu_M$ where the phase is stationary, i.e. where

$$\mathbf{M} \cdot \partial \mathbf{m} / \partial \mu_i = 0 \quad (1 \leqslant i \leqslant f - 1). \tag{3.5}$$

Now each $\partial m/\partial \mu_i$ is a tangent vector on \mathscr{C} , so that (3.5) has the geometric interpretation that the contributions ρ_M come from places μ_M where M is perpendicular to \mathscr{C} (figure 1). In m space such places lie at $m(\mu_M)$ which shall be denoted by m_M . For the convex contours considered here such stationary points can exist only for M in and on the boundary of the positive 'quadrant' and in and on the opposite quadrant, and moreover the signature of the matrix of second derivatives of the exponent of (3.4) is -(f-1). Moreover, some geometry based on (2.7) gives (appendix A)

 $|\nabla U(\mathbf{m}_{\mathbf{M}})| = f/(\mathbf{m}_{\mathbf{M}} \cdot \hat{\mathbf{M}}), \tag{3.6}$

where carats $\hat{}$ will denote unit vectors. The method of stationary phase applied to (3.4) now gives, for M in or on the positive 'quadrant',

$$\rho_{\mathbf{M}}(U) = \frac{\left| \mathbf{m}_{\mathbf{M}} \cdot \mathbf{M} \right|}{\int U^{(f-1)/2f} \left| \mathbf{M} \right|^{\frac{1}{2}(f-1)}} \frac{\exp i[2\pi \mathbf{M} \cdot \mathbf{m}_{\mathbf{M}} U^{1/f} - \frac{1}{4}\pi(f-1)]}{\sqrt{\left| \det \left(\frac{\partial^{2} \mathbf{m} \cdot \hat{\mathbf{M}}}{\partial \mu_{i} \partial \mu_{i}} \right) \right|_{\mathbf{m} = \mathbf{m}_{\mathbf{M}}}}}.$$
(3.7)

The f-1 dimensional determinant is a scalar measure of the *curvature* of \mathscr{C} at m_M . If M is in or on the opposite 'quadrant', ρ is simply given by the complex conjugate of (3.7) for the corresponding point in the positive quadrant. For all other M, ρ_M is zero in this approximation.

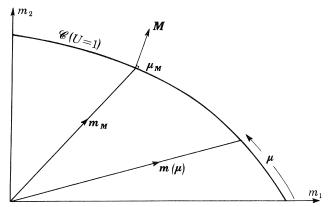


FIGURE 1. Contour $\mathscr{C}(U=1)$ in m space, coordinates μ on \mathscr{C} and the point m_M , where $M \perp \mathscr{C}$, that contributes to the density fluctuation component ρ_M .

In this section so far we have closely followed our earlier study (Berry & Tabor 1976) of the contributions of closed classical orbits to the density of energy levels. Now the argument takes a different turn. Considered as a function of U, $\rho_M(U)$ (equation 3.7) is an oscillation that decays as U increases. This does not mean that ρ_M can be neglected for large U, because the level density which involves the sum of the ρ_M over all M (equation 3.3), always consists of a sequence of delta functions and never tends to its average value of unity no matter how large U becomes.

For very large U the oscillations in ρ_M have almost constant amplitude and wave number over large ranges of U. Thus if

$$U = U_0 + V \quad (U_0 \gg 1, V \ll U_0)$$
 (3.8)

(conditions which permit V to be large compared with unity), (3.7) can be expanded to give the form of the oscillations near U_0 as

$$\rho_{M}(U_{0} + \mathbf{V}) = A_{M}(U_{0}) \exp i(K_{M}(U_{0}) \mathbf{V} + \phi_{M}(U_{0})), \tag{3.9}$$

$$A_{M}(U_{0}) = \frac{|\mathbf{m}_{M} \cdot \hat{\mathbf{M}}|}{\int U_{0}^{(f-1)/2f} |\mathbf{M}|^{\frac{1}{2}(f-1)} \sqrt{\left|\det\left(\frac{\partial^{2} \mathbf{m} \cdot \hat{\mathbf{M}}}{\partial \mu_{i} \partial \mu_{j}}\right)\right|_{\mathbf{m} = \mathbf{m}_{M}}},$$

$$K_{M}(U_{0}) = \frac{2\pi \mathbf{M} \cdot \mathbf{m}_{M}}{\int U_{0}^{1-1/f}},$$

$$\phi_{M}(U_{0}) = 2\pi \mathbf{M} \cdot \mathbf{m}_{M} U_{0}^{1/f} - \frac{1}{4}\pi(f-1).$$

Two things are clear from these expressions: first, a given wavenumber K of the variations of $\rho(U)$ comes from larger terms M as U increases. Secondly, while

where

 K_M and A_M change smoothly as each component of M jumps by unity in the sum (3.3) when U_0 is large, the phase ϕ_M jumps by many times 2π . Therefore $\Delta\rho$ has the character of a random function (Rice 1944, 1945), with a power spectrum

$$\Pi(K) = \sum_{M} A_{M}^{2}(U_{0}) \, \delta(K - K_{M}(U_{0})). \tag{3.11}$$

Elementary methods confirm that $\Pi(K)$ defined this way is identical to the Fourier transform of the autocorrelation function of $\Delta \rho$, i.e.

$$\Pi(K) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dW \, e^{iKW} \, \Delta \overline{\rho(U_0 + V) \, \Delta \rho(U_0 + V + W)}, \tag{3.12}$$

where the average is over V.

The statistical function of interest is not $\Pi(K)$ but the probability distribution P(S) that adjacent levels have spacing S. To relate P and Π , define $g(\Delta) d\Delta$ as the probability of finding a level in the range $U + \Delta$ to $U + \Delta + d\Delta$ given that there is a level at U. Then $g(\Delta)$ is given in terms of the level positions by

$$g(\Delta) = \text{average over all } U(\boldsymbol{m}) \text{ of } \sum_{\boldsymbol{m}' \neq \boldsymbol{m}} \delta(\Delta - (U(\boldsymbol{m}') - U(\boldsymbol{m}))).$$
 (3.13)

It is shown in appendix B that g and Π are related by

$$g(\Delta) = 1 + \int_{-\infty}^{\infty} dK e^{iK\Delta} (\Pi(K) - (1/2\pi)).$$
 (3.14)

Finally, the required level spacing distribution is given in terms of g by (Porter 1965)

$$P(S) = g(S) \exp\left(-\int_0^S g(\Delta) \,d\Delta\right). \tag{3.15}$$

It remains only to evaluate $\Pi(K)$ from (3.11), using the forms (3.10) for $A_M(U_0)$ and $K_M(U_0)$. As $U_0 \to \infty$ these become smooth functions of M, so that the sum in (3.11) can be replaced by an integral over M. When this is done three remarkable things happen. The first is that a simple scaling of M removes the dependence on U_0 ; this shows what is not at all obvious, that the level statistics settle down to a stationary distribution in the classical limit (cf. the beginning of § 5). The second thing is that the same scaling also removes the dependence on K, so that $\Pi(K)$ is a constant, given by

$$\Pi(K) = \frac{1}{f^2} \int \frac{\mathrm{d}^f M(\boldsymbol{m}_M \cdot \hat{\boldsymbol{M}})^2}{|\boldsymbol{M}|^{f-1} \left| \det \left(\frac{\partial^2 \boldsymbol{m} \cdot \hat{\boldsymbol{M}}}{\partial \mu_i \partial \mu_j} \right) \right|_{\boldsymbol{m} = \boldsymbol{m}_M}} \delta \left(1 - 2\pi \frac{\boldsymbol{M} \cdot \boldsymbol{m}_M}{f} \right), \tag{3.16}$$

where the integration is over the positive 'quadrant' only. The third remarkable thing is that this constant is always $1/2\pi$, whatever the shape of the contour U(m) = 1; this is proved in appendix C.

In conjunction with (3.14) these results imply that $g(\Delta)$ is unity, whence (3.15) gives

$$P(S) = e^{-S}. (3.17)$$

For the generic cases to which these methods apply, then, the levels U_m really do arrive at random, and the most probable spacing is zero, indicating strong clustering. This simple-looking result is actually far from trivial in view of the very different behaviour of harmonic oscillators, to be discussed in §§ 5 and 6, and it would not seem likely that (3.17) can be derived in a more elementary way. It is relevant in this connection to remark that in the theory of geometric probability (Kendall & Moran 1963; Hardy & Landau 1924; Hardy 1925), reasoning somewhat similar to ours (i.e. based on the Poisson summation formula) is used to answer questions about the number of lattice points enclosed by circles and ellipses of large radius.

4. THE GENERIC CASE: NUMERICAL EXPERIMENTS

Given any 'Hamiltonian' U(m), it is an easy matter to compute all levels m for which U(m) is less than some large number U_{max} , arrange them in order of increasing U, compute the differences S between the U-values of adjacent levels and plot the spacing distribution P(S) as a histogram. In our experiments we first took $U_{\text{max}} = 5000$ and then repeated the calculations with $U_{\text{max}} = 10000$, to check that the distributions P(S) were stable (they were, in every case except one which will be mentioned in § 6).

The first experiments were with two-dimensional boxes (case II of § 2) with sides a_1 and a_2 ; setting $a_1^2/a_2^2 \equiv a/b$ equation (2.11) gives

$$U^{II}(\mathbf{m}) = \frac{1}{4}\pi (m_1^2 \sqrt{(b/a)} + m_2^2 \sqrt{(a/b)}). \tag{4.1}$$

Figure 2a shows P(S) for $a/b = \sqrt{2}$. The exponential distribution (3.17) is clearly a good fit. Calculations for $a/b = \sqrt{3}$, $\sqrt{5}$, $\sqrt{7}$ and $\frac{1}{2}(\sqrt{5}-1)$ show essentially the same behaviour and will not be presented here.

If a and b are integers such that the fraction a/b is in its lowest terms, (4.1) shows that all levels and therefore all level spacings S must be integer multiples of $X \equiv \pi/4\sqrt{(ab)}$. This means that (3.17) cannot be correct as it stands, but could still hold if interpreted to mean that the probability of spacing nX is

$$P(n) = (1 - e^{-X})e^{-nX}. (4.2)$$

The experiments do seem to confirm this: figure 2b shows P(S) for $a/b = \frac{5}{7}$, and it can be seen that again the exponential gives a good fit. This applies also to the case a/b = 1 (not shown), while a/b = 1.01 gives a smooth exponential distribution like that on figure 2a.

The physical difference between a/b rational and irrational is that in the former case the classical orbits picked out by the quantum condition are all closed and in the latter case never closed; this is not a generic property of the regular spectrum.

In the second set of experiments, the 'boxed oscillator' (case III of § 2) was studied. $U(\boldsymbol{m})$ is given by equation (2.13) and depends on the energy E through the parameter $K \equiv 4E_{\beta}/\alpha^2$. (4.3)

P(S) was computed for K = 0.002, 2 and 2000. In all cases the description was closely exponential as shown by figure 3, which is drawn for the case K = 2.

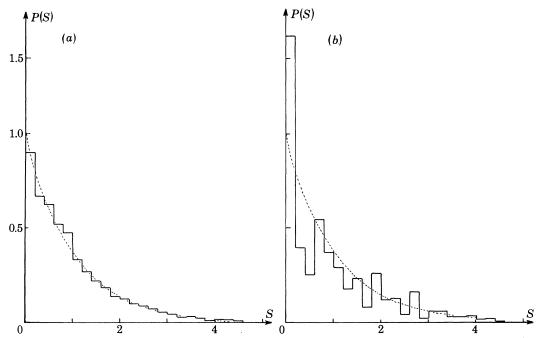


FIGURE 2. Distributions of spacings of lowest 5000 levels for particles in two-dimensional boxes with side ratio a^2/b^2 where (a) $a/b = \sqrt{2}$ (b) $a/b = \frac{5}{7}$. The dotted lines show the exponential distribution.

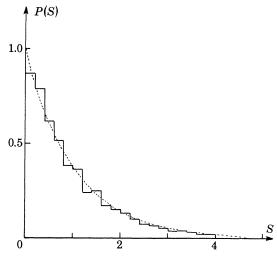


Figure 3. Distribution of spacings of lowest 50000 levels for two dimensional 'boxed oscillator' (equations 2.13 and 4.3) with K=2. The dotted line shows the exponential distribution.

5. HARMONIC OSCILLATORS: THEORY

For these systems (case I of § 2) the contours $U^{I}(\mathbf{m}) = \text{constant}$ are flat (equation 2.9). To show what a dramatic effect this has on the level spacings, consider first the case when the frequencies ω are rationally related. Then ω , considered as a vector in \mathbf{m} space, has a rational direction, and may be written

$$\omega = N\omega_0, \tag{5.1}$$

where N is a vector of relatively prime non-negative integers. In m space all lattice points lie on lattice planes which can be chosen normal to N. But the contours U= constant are planes normal to ω (equation 2.9) and therefore pass through these lattice planes as U increases. Therefore these rational oscillator levels are degenerate, the degeneracy at each passage of a U contour through a lattice plane being equal to the number of lattice points on the part of the plane lying in and on the positive 'quadrant' in m space. This number is greater for lattice planes farther from m=0, so that the degeneracy of the levels increases with U. Of course, the average level density $\bar{\rho}$ has to remain unity, so that the spacing of these increasingly degenerate levels gets larger as U increases.

This behaviour is quite complicated for general N, but can be understood in detail for the simplest case $N = \{1, 1, ..., 1\}$. Then the lth degenerate level lies at $U = l^{f}/f!$ and has a degeneracy a_{l} equal to the number of permutations of f nonnegative integers whose sum is l. Therefore the level density is

$$\rho(U) = \sum_{l=0}^{\infty} a_l \delta(U - (l^f/f!)).$$
 (5.2)

 a_l is also the number of points in the lth lattice plane normal to $\{1, 1, ..., 1\}$; the leading term for large l, which underestimates the contribution from lattice points on the boundary of the positive 'quadrant', is

$$a_l \rightarrow l^{f-1}/(f-1)!$$
 as $l \rightarrow \infty$, (5.3)

from which it is clear that $\bar{\rho}$ is indeed unity for (5.2).

The important point here is that this behaviour is in no way stochastic: the levels arrive ever more pathologically in the classical limit, and no spacing distribution P(S) exists. This is in marked contrast with the generic case discussed in § 3, where levels arrived at random in the classical limit. In fact the argument given there cannot be applied to harmonic oscillators. Of course the Poisson summation formula can still be employed, and the quantities $\rho_M(U)$ (equation 3.4) introduced; it is the method of stationary phase that is inapplicable. The reason is that for flat contours U = constant, the stationary phase condition (3.5) (M normal to contour) is satisfied either at all points on the contour (rationally related components of ω) or at no point on the contour (irrationally related components of ω). Isolated stationary points never occur.

Ignoring the case of partial commensurability of the frequencies ω , which can occur when f > 2, we still have to consider the totally irrational oscillators, where

no two components of ω are commensurable. Then the vector ω never intersects a lattice point m (except the origin) even when extended to infinity, so that none of the contours of U (normal to ω) are lattice planes. Therefore no degeneracies can occur in this case. However, it is possible to choose lattice planes whose normals N are arbitrarily close 'rational approximations' to ω , and this leads us to expect

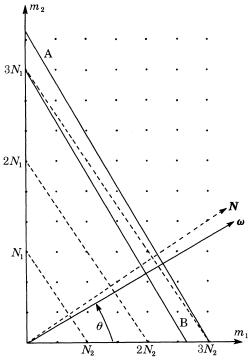


FIGURE 4. Irrational frequency vector ω and close rational approximation $N = \{3, 2\}$. The dotted lines $\perp N$ are the lattice planes containing 2, 3 and 4 points and the full lines A and B are the contours for which $U = U(3N_2, 0)$ and $U = U(0, 3N_1)$.

that when the U contour passes through such a plane, all of its points will be intersected in quick succession, giving a near-degeneracy, a dense cluster of levels so that the spacing distribution P(S) might have a large value at S=0, as in the generic cases previously discussed. It was a surprise to discover that this is not the case: for large U there is no level clustering for irrational oscillators!

To explain this we restrict ourselves to the two-dimensional case, where the lattice 'planes' are lines and the irrational ratio is

$$\omega_2/\omega_1 \equiv \alpha \equiv \tan \theta, \tag{5.4}$$

and without loss of generality we can take $\alpha < 1$. Then ω makes an angle θ with the m_1 axis (figure 4). Now choose N, the normal to a set of lattice lines approximately parallel to ω , i.e.

$$N_2/N_1 \approx \alpha.$$
 (5.5)

Then the lattice line that intersects the axes m_1 and m_2 at points $(\nu N_2, 0)$ and $(0, \nu N_1)$ (figure 4), will contain $\nu + 1$ points m. The level position corresponding to each such point is, from (2.9)

$$U(\mathbf{m}) = (m_1 \cos \theta + m_2 \sin \theta)^2 / \sin 2\theta = \frac{1}{2} (m_1 / \sqrt{\alpha + m_2 / \alpha})^2$$
 (5.6)

and the mean spacing in this group of $\nu + 1$ levels is

$$\Delta U \equiv \left| (1/\nu + 1) \left[U(0, \nu N_1) - U(\nu N_2, 0) \right] \right|
= \left| \frac{\nu^2 (N_1^2 \sin^2 \theta - N_2^2 \cos^2 \theta)}{(\nu + 1) \sin 2\theta} \right|
\approx \nu N_1^2 |\alpha - N_2/N_1|,$$
(5.7)

the approximate equality being obtained by use of (5.5).

But because ΔU increases with ν this calculation shows that the increase in the number $\nu+1$ of levels in each group as U increases is not a source of level clustering – its effect is outweighed by the 'slowing down in the rate of recession' of the contours of U from the origin as U increases (this 'rate' is proportional to $U^{1/f-1}$). The only remaining possibility of clustering lies in taking $\nu=1$ (groups of just two levels) and seeking ever closer rational approximations N_2/N_1 to α .

Now the best sequence of rational approximations to α is obtained in terms of the successive convergents of its *simple continued fraction*. This is

$$\alpha = \underbrace{\frac{1}{a_1 + \underbrace{1}{a_2 + \underbrace{1}{a_3 + \ddots}}}} \equiv [a_1 \, a_2 \, a_3 \, \dots], \tag{5.8}$$

where the quantities a_i are positive integers, uniquely defined by the integral parts of the successive reciprocals of the non-integral parts of α . The successive convergents are the rational fractions

$$p_k/q_k = [a_1 \, a_2 \, a_3 \dots a_k]. \tag{5.9}$$

They are best approximations to α in the sense that no rational fraction p/q with $q \leq q_k$ lies closer to α than p_k/q_k . This is proved in all texts on arithmetic, e.g. the classic by Khinchin (1964) or the more modern presentation by Drobot (1964). A physical interpretation of this result is given by Klein (1932): if pegs are attached to each lattice point m and the vector ω replaced by a taut infinite string with one end fixed at infinity and the other end free at m=0, then the pegs snagged by the string as the free end is moved first to one side and then to the other have coordinates $m=(q_k,p_k)$.

It follows that in our search for level clustering we can do no better than study those lattice planes whose normals N are (q_k, p_k) . It is an algebraic consequence of (5.8) and (5.9) that $|\alpha - p_k/q_k| < 1/q_k q_{k+1}$. (5.10)

Therefore the level spacing ΔU (5.7 with $\nu = 1$) satisfies

$$\Delta U < q_k / q_{k+1} \equiv C_k \tag{5.11}$$

as k increases and α is ever more closely approximated. The bounds C_k must be less than unity, because the denominators of the convergents increase with k (It is worth pointing out that if the 'decimal' expansion of α to base b is employed instead of the continued fraction, C_k is of order b^k , so that 'decimal' approximations are quite hopeless as a means of generating level clustering.)

For any α whatever, it is shown in the works cited that the smallest value of C_k for which (5.11) is guaranteed to hold for an infinite number of convergents α is $1/\sqrt{5}$. This implies that in general clustering does not occur as α is better and better approximated. If certain classes of 'more irrational' α are excluded, however, C_k can be reduced. For example, if the 'most irrational number', namely

$$\alpha = [1, 1, 1, 1, \dots] = \frac{1}{2}(\sqrt{5} - 1) = \text{'golden number'}$$
 (5.12)

is excluded, as well as all numbers for which the sequence of integers (5.8) ends in an infinite sequence of 1s, C_k can be reduced from $1/\sqrt{5}$ to $1/\sqrt{8}$. If all quadratic irrationals (i.e. those α satisfying a quadratic equation with integer coefficients) are excluded C_k comes down to $\frac{1}{3}$, while the exclusion of all algebraic irrationals reduces C_k further, to a quantity which however is still a constant of order unity.

This still fails to give clustering, which requires C_k to be a decreasing function of k (e.g. e^{-k} , or q_k^{-4}). For any such function C_k , however, it is known that a class of α can always be found which satisfies (5.11) for an infinite number of ks. Such numbers are transcendental and lie closer to rationals than algebraic irrationals. Harmonic oscillators with these frequency ratios might at last show clustering. It is not possible to be more precise, because it is still not known what function C_k corresponds to any given transcendental number such as e or π . But it is possible to conjecture an answer to the following question: will a 'generic' harmonic oscillator system exhibit clustering? The generic oscillator will of course have irrational α , since the rationals are infinitely sparse among the reals, and it will also have transcendental α , since the algebraic irrationals, being countable, are also infinitely sparse among the reals. This does not imply clustering, since not all transcendentals have decreasing C_k s. Indeed it was shown by Lévy (see Khinchin 1964) that for 'almost all' α (in the sense of measure theory), the denominators q_k increase as

$$(q_k) \xrightarrow{k \to \infty} (e^{\pi^2/12 \ln 2})^k. \tag{5.13}$$

This astonishing result suggests that in the typical case the bound C_k in (5.11) has the limit

$$C_k \xrightarrow{k \to \infty} e^{-\pi^2/12 \ln 2} \approx 0.305. \tag{5.14}$$

Since this is a constant, it seems that there is no level clustering for generic oscillators. In view of the inevitable inaccuracy of physical measurements and the consequent impossibility of ascertaining the arithmetic nature of the frequency ratio for any real oscillator, it is perhaps this result about the 'typical' oscillator that is of most physical significance.

In the theory of geometric probability (Kendall & Moran 1963; Hardy & Littlewood 1922) the number of lattice points enclosed by a large right triangle with

angle θ is studied; continued fractions are employed in this work, and it is found that the results depend crucially on the arithmetic nature of tan θ , but the problems of clustering that are our particular concern here are not considered.

We have not been able to prove for any irrational oscillator that the level spacings settle into a stable distribution P(S) as $U \to \infty$. If they do (as the numerical experiments of § 6 seem to indicate) then our arguments about the absence of clustering for generic oscillators suggest that P(S) should reach its maximum away from S=0, in sharp contrast with the behaviour of fully generic regular systems.

In physical terms, the levels will be distributed more regularly for irrational oscillators than for the systems considered in §§ 3 and 4. It is likely that P(S) for some transcendental oscillators (which may have a greater propensity towards clustering) will be less concentrated about the mean value of unity than P(S) for oscillators with merely algebraic irrationality.

The arguments of this section and § 3 lead to an interesting question of limits. Suppose that a generic regular system (curved U contours), depends on two parameters δ and ϵ in such a way that as $\delta \to 0$ the system degenerates into an irrational oscillator and that if then $\epsilon \to 0$ the system degenerates further into a rational oscillator. It would seem that as $\delta \to 0$ P(S) should change discontinuously from an exponential to a peaked distribution and then, as $\epsilon \to 0$, to no distribution at all! This is not the case. For small but finite ϵ and δ the lowest levels consist of tight clusters whose spacings and populations increase with U. For larger U these clusters open up (cf. the factor ν in 5.7) and the levels adopt the relatively regular distribution characteristic of irrational oscillators. Finally, at even greater values of U the regularity gradually gets replaced by the random distribution characteristic of generic systems; this will be demonstrated numerically in the next section. (In mathematical terms the slightest curvature of the contour U=1 will, for sufficiently large U, cause the integrand in (3.4) to oscillate rapidly enough to justify the method of stationary phase.)

6. HARMONIC OSCILLATORS: NUMERICAL EXPERIMENTS

Values of U(m) were calculated for irrational values of α from equation (5.6) and histograms constructed for the spacing distribution P(S). Figure 5a shows P(S) for $\alpha = 1\sqrt{2}$. The distribution is tightly peaked about S = 1 showing the expected absence of clustering in comparison with the generic cases of figures 2 and 3. The other quadratic irrationals $\alpha = 1/\sqrt{3}$, $1/\sqrt{7}$ and $\frac{1}{2}(\sqrt{5}-1)$ show essentially the same behaviour. The case $\alpha = 1/\sqrt{5}$ (figure 5b) seemed exceptional at first in that the spacings of the lowest 5000 levels were distributed bimodally; however, when the lowest 10000 levels were taken P(S) settled into a form similar to that for the other quadratic irrationals. None of these distributions is well fitted by the Wigner distribution $P_{\text{Wigner}}(S) = \frac{1}{2}\pi S \, \mathrm{e}^{-\frac{1}{4}\pi S^2}, \tag{6.1}$

which gives such an accurate description of the spacings of levels of complex nuclei (Porter 1965).

Next P(S) was computed for the transcendental frequency ratio $\alpha = \pi^{-1}$. This time the distribution was bimodal with a strong tight peak near $S = \frac{1}{2}$ and a weak broad peak near S = 4.3; this distribution was already fully evident in the lowest 5000 levels, and hardly changed when 10000 levels were taken (figure 6a). In view of the arguments of the last section this is not too surprising. π is rather 'close' to many rational numbers; for example the third convergent, namely

$$p_3/q_3 = 355/113,\tag{6.2}$$

approximates π with a fractional error of order 10^{-7} . Therefore the bounds C_k (equation 5.11) decrease rapidly with k, at least for small k, and some degree of clustering is to be expected.

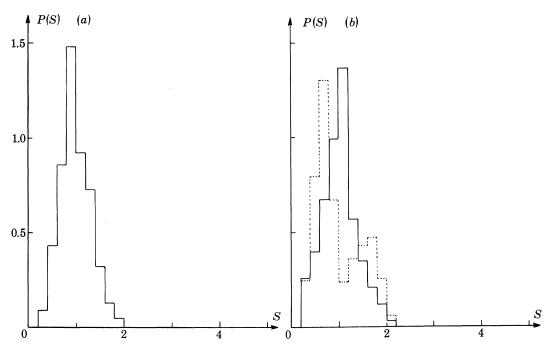


FIGURE 5. Level spacing distributions for two-dimensional harmonic oscillators with frequency ratio α . (a) $\alpha = 1/\sqrt{2}$, lowest 5000 levels (b) $\alpha = 1/\sqrt{5}$, lowest 5000 levels (dotted line), lowest 10000 levels (full line).

However, not all transcendental oscillators behave in this way. Figure 6b shows P(S) for the lowest 10 000 levels of the oscillator with $\alpha=\mathrm{e}^{-1}$. The distribution is tightly peaked about S=1, just as in the case of quadratic irrationals, the only difference being a hint of a large-S tail with some spacings of S=2.4, a value not attained by any quadratically irrational oscillator. This absence of clustering accords with our conjecture based on (5.4) about the behaviour of generic irrational oscillators.

The final series of computations illustrates the transition discussed at the end

of § 5, from a peaked to an exponential distribution P(S) as U increases for a system whose contours U(m) = constant are almost flat. The system is the 'perturbed oscillator' (case IV of § 2) whose 'Hamiltonian' is given by (2.15). Figures 7a-d show the distributions, as increasing numbers of levels are taken into account, for the oscillator with frequency ratio $\omega_1/\omega_2 = 1/\sqrt{2}$ and perturbation $\epsilon = 0.005$.

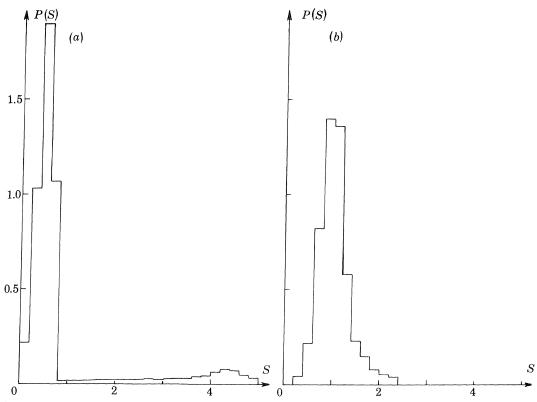


Figure 6. Distribution of spacings of lowest 10 000 levels for two-dimensional harmonic oscillators with frequency ratio (a) $\alpha = \pi^{-1}$, (b) $\alpha = e^{-1}$.

For U=1000 (figure 7a) the maximum of P(S) is still near S=1 as for typical irrational oscillators, but there is already some clustering, revealed by the fact that $P(0) \neq 0$. This shows the extreme sensitivity of oscillator systems, since the perturbation ϵ is so small that the curvature of any contour U= constant amounts only to a change in direction of about $\frac{1}{4}$ ° along its whole length. Including the lowest 2000 levels (figure 7b) has almost eliminated the peak in P(S). By U=5000 (figure 7c) the peak has gone completely, and by U=7500 P(S) closely approximates the exponential form characteristic of generic regular spectra. The same limiting distribution was obtained by perturbing the rational oscillator with $\omega_1/\omega_2=1$.

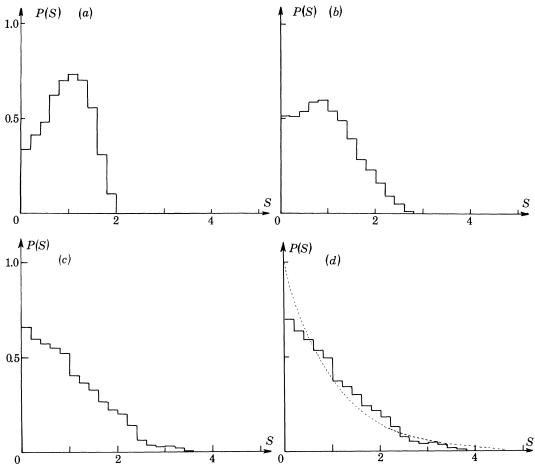


FIGURE 7. Level spacing distributions for perturbed oscillator system (equation 2.15), with $\omega_1/\omega_2=1/\sqrt{2}$ and $\epsilon=0.005$, including the lowest $U_{\rm max}$ levels, where (a) $U_{\rm max}=1000$, (b) $U_{\rm max}=2000$, (c) $U_{\rm max}=5000$, (d) $U_{\rm max}=7500$. On (d) the exponential distribution is shown as a dotted line.

7. Conclusions

Using a combination of theory, conjecture and numerical experiment we have explored the correlations between neighbouring energy levels in the regular spectrum, with the following surprising result: although in the generic case where the energy contours in action space are curved, the level spacing distribution has the exponential form characteristic of a purely random process, in the case of harmonic oscillators with incommensurable frequencies, P(S) is sharply peaked, indicating a more regular distribution of levels, the precise nature of which depends on the arithmetic nature of the frequency ratios. If the oscillators have commensurable frequencies, P(S) does not exist.

What is the experimental significance of these results? At present there is none,

because the correspondence principle implies (Percival 1973) that in the semiclassical limit each regular level is coupled by (non-pathological) perturbations only to those with neighbouring vector quantum numbers m and not to those with similar energy and very different m. This rules out any attempt to measure P(S)by exciting a given level and observing the spectrum produced by its decay.

This situation will change if Percival's irregular spectrum is discovered. Then P(S) would be a measurable function, because each irregular level is expected to be weakly coupled to all other irregular levels with similar energy, and the low frequency part of the spectrum produced when a single irregular level is excited (e.g. by a laser if the system is an asymmetrical vibrating molecule) would depend strongly on P(S) (more precisely the spectrum would depend on $g(\Delta)$ defined in 3.13).

Of course the distributions P(S) for irregular systems need not be any of those discussed here, which apply to regular systems. However, it is now known (Arnold & Avez 1968) that generic classical systems are neither purely integrable (regular) nor ergodic (irregular), but exhibit a most intricate combination of these two forms of behaviour, with some orbits being confined to f-dimensional manifolds in the 2f-dimensional phase space (i.e. acting as though f constants of motion existed) and other orbits with infinitesimally different initial conditions not being so confined. The semi-classical quantum theory of these systems has not been developed. Any such theory must be capable of predicting energy level spacing distributions. It is obviously necessary to begin by studying such distributions for the simplest cases, namely regular systems, and that is what we have tried to do in this paper.

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APPENDIX A

This is the proof of (3.6). $|\nabla U|$ has to be evaluated at m_M on the contour U=1. At the point $(1+\epsilon)m_M$, the scaling (2.7) gives, for the change in U when $\epsilon \to 0$,

$$dU \equiv U((1+\epsilon) \, \mathbf{m}_{\mathbf{M}}) - 1 = (1+\epsilon)^f \times 1 - 1 \simeq \epsilon f. \tag{A 1}$$

The normal distance dl between the contours U = 1 and U = 1 + dU is

$$dl = \epsilon \mathbf{m}_{\mathbf{M}} \cdot \hat{\mathbf{M}}, \tag{A 2}$$

so that the gradient of U is

$$|\nabla U| = \frac{\mathrm{d}U}{\mathrm{d}l} = \frac{\epsilon f}{\epsilon m_M \cdot \hat{M}}$$
 (Q.E.D.) (A 3)

APPENDIX B

This is the proof that $g(\Delta)$ (3.13) and $\Pi(K)$ (3.12) are related by (3.14). Substitution of (3.12) into (3.14) gives

$$g(\Delta) = 1 - \delta(\Delta) + \overline{\Delta\rho(U_0 + V)\,\Delta\rho(U_0 + V + \Delta)}.$$
 (B 1)

From (3.2) and (2.5)

$$\Delta \rho(U) = \sum_{m} \delta(U - U(m)) - 1$$
 (B 2)

substitution into B 1 and use of the fact that $\bar{\rho} = 1$ gives

$$g(\Delta) = -\delta(\Delta) + \overline{\sum_{\substack{m_1 m_2 \\ m_1 m_2}} \delta(U_0 + V - U(m_1)) \delta(U_0 + V + \Delta - U(m_2))}.$$
 (B 3)

The term $-\delta(\Delta)$ is cancelled by the terms $m_1 = m_2$, leaving

$$g(\Delta) = \sum_{m_1} \overline{\delta(U_0 + V - U(\boldsymbol{m_1}))} \sum_{m_2 + m_1} \delta(\Delta - (U(\boldsymbol{m_2}) - U(\boldsymbol{m_1}))). \tag{B 4}$$

The average, taken over some great range L of V containing N=L levels, can be written as

$$\sum_{m_1} \overline{\delta(U_0 + V - U(m_1))} = \frac{1}{L} \int_{-\frac{1}{2}L}^{\frac{1}{2}L} dV \sum_{m_1} \delta(U_0 + V - U(m_1))$$

$$= \frac{1}{N} \sum_{\substack{m_1 \text{ for which} \\ U_0 - \frac{1}{2}L < U(m_1) < U_0 + \frac{1}{2}L}} = \text{average over all } U(m), \quad (B.5)$$

so that (B 4) becomes identical with (3.13) (Q.E.D.).

APPENDIX C

This is the proof that the R.H.S. of (3.16) equals $\frac{1}{2}\pi$. Denote |M| by M and \hat{M} by Ω . Then the integral over M in (3.16) removes the delta function, to give

$$H(K) = \frac{1}{2\pi f} \int \frac{\mathrm{d}^{f-1}\Omega |\boldsymbol{m}_{M} \cdot \boldsymbol{\Omega}|}{\left| \det \left(\frac{\partial^{2} \boldsymbol{m} \cdot \boldsymbol{\Omega}}{\partial \mu_{i} \partial \mu_{j}} \right) \right|_{\boldsymbol{m} = \boldsymbol{m}_{M}}}.$$
 (C 1)

Now denote $|m_M|$ by m and \hat{m}_M by ω . As M varies, m_M will vary too (figure 1) so that it is possible to change variables from Ω to ω in C 1 to give an integral over the contour U = 1 whose polar equation is $m = m(\omega)$:

$$\Pi(K) = \frac{1}{2\pi f} \frac{\int \mathrm{d}^{f-1}\omega |\partial \mathbf{\Omega}/\partial \omega| m\omega \cdot \mathbf{\Omega}}{\left| \det \left(\mathbf{\Omega} \cdot \frac{\partial^2 m\omega}{\partial \mu_i \partial \mu_j} \right) \right|}.$$
 (C 2)

If now local cartesians $\eta = \{\eta_1 \dots \eta_{f-1}\}$ are introduced in the tangent hyperplane to the contour at ω , instead of the curvilinear coordinates μ , then

$$\left| \det \left(\mathbf{\Omega} \cdot \frac{\partial^2 m \boldsymbol{\omega}}{\partial \mu_i \, \partial \mu_i} \right) \right| = \left| \det \left(\frac{\partial \Omega_i}{\partial \eta_i} \right) \right| = \left| \frac{\partial \mathbf{\Omega}}{\partial \boldsymbol{\eta}} \right|. \tag{C 3}$$

Thus (C 2) becomes

$$\Pi(K) = \frac{1}{2\pi f} \int d^{f-1}\omega m(\boldsymbol{\omega} \cdot \boldsymbol{\Omega}) \left| \frac{d\boldsymbol{\eta}}{d\boldsymbol{\omega}} \right|. \tag{C 4}$$

Now projecting along ω the element of tangential hyperarea $d\eta$, whose normal lies along Ω , gives an area element normal to ω , i.e.

$$|\mathrm{d}\boldsymbol{\eta}|\boldsymbol{\omega}\cdot\boldsymbol{\Omega}=m^{f-1}|\mathrm{d}\boldsymbol{\omega}|,\tag{C 5}$$

so that

$$\Pi(K) = \frac{1}{2\pi} \left[\frac{1}{f} \int d^{f-1} \omega m^f(\omega) \right]. \tag{C 6}$$

But the quantity in square brackets is just the hypervolume of the positive 'quadrant' enclosed by the contour U=1, and this is just unity. Therefore $H(K)=\frac{1}{2}\pi$ (Q.E.D.).