Arithmetical degeneracies in simple quantum systems

1986 J. Phys. A: Math. Gen. 19 211

(http://iopscience.iop.org/0305-4470/19/2/017)

J. Phys. A: Math. Gen. 19 (1986) 211-239. Printed in Great Britain

Arithmetical degeneracies in simple quantum systems

C Itzykson and J M Luck

Service de Physique Théorique, CEN Saclay, BP2, 91191 Gif-sur-Yvette, Cedex, France

Received 22 May 1985

Abstract. We examine the 'accidental' level degeneracies occurring in the quantum mechanical problem of a free particle moving in a polyhedral box, when the problem is integrable. Some remarkable properties of the distribution of degeneracies are studied in several two-, three- and four-dimensional examples and are related to well known problems of number theory. The numerical results of exact enumerations are compared with analytical predictions, or with conjectured expressions in some cases. We consider in particular the asymptotic scaling form of the degeneracy distribution up to some maximal energy E, and the maximal degeneracy occurring for energies less than some given E.

1. Introduction

Simple quantum systems can exhibit unexpected features. We focus here on the spectrum of the Hamiltonian for a particle moving freely in a box, when the problem is integrable. This is a classroom example in any elementary exposition of wave mechanics. As Rayleigh observed [1], when discussing rectangular vibrating membranes (with sides a and b): 'when a^2 and b^2 are commensurable ... the specification of the period does not completely determine the type. The full consideration of the problem ... requires the aid of the theory of numbers'.

The question of 'accidental' degeneracies has recently been revived in the physics literature by Berry [2]. A review of the Dirichlet problem is given by Kuttler and Sigillito [3], while the case of an equilateral triangular box is discussed by Pinsky [4].

The usual arguments in quantum mechanics suggest that degeneracies occur due to symmetries, whether manifest or 'hidden', with an associated group theoretical framework. This would, for instance, apply to the spectrum of a particle constrained to move on a sphere, but otherwise free. The accidental degeneracies do not seem to follow the same pattern, very much as the distribution of prime numbers cannot be described using an 'elementary' construction process. We shall see that this property is shared by the distribution of degeneracies in the examples that we shall study. This close relationship to number theory is at first somehow unexpected.

The mathematical literature on these topics is abundant. In due course we shall quote a rather eclectic list of texts that we found useful, without any pretence at completeness nor accuracy—a measure of our ignorance.

Take for instance the case of a particle in a two-dimensional square box of size a. In units of $\hbar^2\pi^2/2ma^2$ the energy levels are the sums of two positive integers, and hence are themselves positive integers. Counting the points with integral coordinates inside a large circle, one deduces that the asymptotic density of levels is $\pi/4$, i.e. slightly smaller than one. It is somehow surprising to discover [2] that the fraction of integers belonging to the spectrum up to a maximal value E vanishes as $(\ln E)^{-1/2}$ when E tends to infinity. This, however, is not in contradiction with the asymptotic expansion for the integrated density of states, as developed in the general case by Balian and Bloch [5], as we shall see through examples. In three dimensions, for a cubic box, the density of states grows like $2\pi E^{1/2}$. But it turns out that asymptotically one-sixth of the integers do not belong to the spectrum. Fermat stated, and Euler and Lagrange proved [6], that such vacancies do not occur in dimension four or greater.

Our aim is to present these and similar results with a minimal appeal to number theory and to show relationships between similar systems. In the first part we review some classical material on the integrable cases of the Dirichlet problem (§ 2) and related number theoretical identities (§ 3). Rather than discussing these identities in a pure arithmetical context, we have chosen to relate them to elementary quantum statistical problems. We obtain in particular a straightforward derivation of Jacobi's triple product identity. In the second part (§ 4) we study the modes for a square or equilateral triangular box, a problem investigated by Lamé around 1850. The mathematical tools are Dirichlet series which generalise Riemann's ζ function. We show that the kth moment of the distribution of degeneracies up to some energy E scales like $(\ln E)^{2^{k-1}-1}$, a result valid both for the square and equilateral triangle, and study some related aspects of this distribution.

In the third part (§ 5) we look at three- and four-dimensional examples. We exhibit the finite lacunarity of the spectrum in three dimensions and conjecture the existence of a scaling form of the distribution of degeneracies in dimension three and higher.

The theoretical predictions can be checked against numerical evidence. The latter also allows in certain cases an estimate of the errors. The values of the largest energies required to exhibit the trend to asymptotes strongly depend on the quantity under consideration. To obtain the data is quite easy using computer facilities for systematic enumeration. For instance, in figure 6 we plot values of E in reduced units up to 2×10^7, but certain phenomena are already apparent for much smaller values, such as the Balian-Bloch oscillations or the finite lacunarity in three dimensions, where a maximal energy of a few hundreds is sufficient. A complete theory of the subdominant terms would lead us too far astray, into the realm of Riemann's hypothesis.

In the final section (§ 6) we speculate on the relation between degeneracies and sensitivity to perturbations and suggest further lines of inquiry.

An appendix gives an elementary, albeit technical, proof of some formulae needed to compute the mode degeneracies in an equilateral triangular box or its cartesian square.

2. Free particle in a box

A free particle moving inside a box B in a Euclidean space of dimension d, with energy E, satisfies Schrödinger's equation in the form

$$\left(\frac{\hbar^2}{2m}\Delta + E\right)\Psi(x) = 0 \qquad \Psi(x)|_{x\in\partial B} = 0. \tag{2.1}$$

This is Dirichlet's problem. We assume the box to be compact and bounded by finitely many plane walls. Applying the method of images, or Schwarz's reflection principle, the problem is integrable when the group generated by the reflections in the walls provides a 'tiling' of all space. Such groups have been classified by Coxeter [7] and are related to the classification of semi-simple Lie algebras according to Cartan and Weyl. In such a case the wavefunctions and energy levels can be obtained explicitly using finite superpositions of plane waves according to the corresponding symmetry group. Integrability does not necessarily mean separability. The latter applies when the box can be identified with a cartesian product of boxes in orthogonal subspaces. Richens and Berry [8] have coined the word 'pseudo-integrable' for the case when the dihedral angles of the box are fractional multiples of π but the group of reflections fails to give a tiling of space. We hope to return to this case in a future paper.

The simplest example is a two-dimensional rectangular box of sides a and b, a separable case. With n_1 and n_2 positive integers, the wavefunctions and energies are

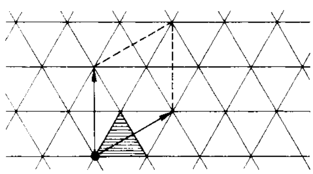
$$\Psi_{n_1,n_2}(x, y) = \sin(n_1 \pi x/a) \sin(n_2 \pi y/b) \qquad E = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_1^2}{a^2}+\frac{n_2^2}{b^2}\right). \tag{2.2}$$

As the simplest commensurate case we shall limit ourselves to a square

$$a = b \qquad E = \frac{\hbar^2\pi^2}{2ma^2}(n_1^2+n_2^2) \qquad n_1, n_2 > 0. \tag{2.3}$$

One could also look at a triangle with angles $(\pi/2, \pi/4, \pi/4)$ obtained by cutting the square in half along a diagonal. The corresponding eigenfunctions are obtained by antisymmetrising the previous ones in the interchange $x \Leftrightarrow y$, and the energy levels are the same, except for the restriction $n_1 > n_2$.

The construction of the solutions in the equilateral triangle case [4-9] illustrates the general principles [10], so we shall repeat it here in some detail. The reflections in the walls of an equilateral triangle of side a generate a triangular lattice. The translation subgroup is generated by the periods $a(1-j^2)$, $a(j-j^2)$, where $j = \exp(\mathrm{i}2\pi/3)$ (see figure 1(a)). Through the origin we have a representative of each family of parallel walls. Denote by R_1, R_2, R_3 the reflections through each of them,



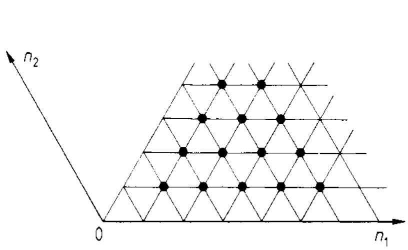


Figure 1. (a) The equilateral triangle and two fundamental periods. (b) Representative points of the states in momentum space.

and parametrise a point in the plane using the complex number $z=x+jy$. A fundamental domain is $0\leqslant y\leqslant x$ and the Laplacian reads

$$z=x+jy \qquad \Delta=\tfrac{4}{3}(\partial_x^2+\partial_y^2+\partial_{xy}^2). \tag{2.4}$$

The point group generated by R_1, R_2, R_3 is isomorphic to the permutation group on three objects S_3. Applying to any differentiable function $\varphi(\boldsymbol{x})$ the operator $A\varphi(\boldsymbol{x})=\Sigma_{\gamma\in S_3}(-1)^\gamma\varphi(\gamma\boldsymbol{x})$, we obtain a similar function vanishing on the three lines (i) $y=0$, (ii) $x=0$, (iii) $x=y$. In the following table we list γ, $(-1)^\gamma\varphi(\gamma\boldsymbol{x})$ and the phase factor resulting from increasing $x\to x+a$, or $y\to y+a$ for a plane wave $\varphi(\boldsymbol{x})$ of the form $\exp[\mathrm{i}(2\pi/a)(Mx+Ny)]$, where M and N are left unspecified, and $L=-(M+N)$.

γ	$(-1)^\gamma\varphi(\gamma\boldsymbol{x})$	$x\to x+a$	$y\to y+a$
1	$\exp[(2\pi\mathrm{i}/a)(Mx+Ny)]$	$\exp(2\pi\mathrm{i}\,M)$	$\exp(2\pi\mathrm{i}\,N)$
R_1	$-\exp[(2\pi\mathrm{i}/a)(Mx+Ly)]$	$\exp(2\pi\mathrm{i}\,M)$	$\exp(2\pi\mathrm{i}\,L)$
R_2R_1	$\exp[(2\pi\mathrm{i}/a)(Lx+My)]$	$\exp(2\pi\mathrm{i}\,L)$	$\exp(2\pi\mathrm{i}\,M)$
R_2	$-\exp[(2\pi\mathrm{i}/a)(Lx+Ny)]$	$\exp(2\pi\mathrm{i}\,L)$	$\exp(2\pi\mathrm{i}\,N)$
R_1R_2	$\exp[(2\pi\mathrm{i}/a)(Nx+Ly)]$	$\exp(2\pi\mathrm{i}\,N)$	$\exp(2\pi\mathrm{i}\,L)$
R_3	$-\exp[(2\pi\mathrm{i}/a)(Nx+My)]$	$\exp(2\pi\mathrm{i}\,N)$	$\exp(2\pi\mathrm{i}\,M)$

The choice

$$\exp(2\pi\mathrm{i}\,M)=\exp(2\pi\mathrm{i}\,N)=\exp(2\pi\mathrm{i}\,L)=\exp(\mathrm{i}\alpha) \tag{2.5}$$

ensures that $\Psi=A\varphi$ is a solution of Schrödinger's equation in the complete plane and vanishes on the three families of parallel walls, i.e. it is a solution in a triangular box, and one can show that all solutions have been obtained. From equation (2.5)

$$\Psi(x+a,y)=\Psi(x,y+a)=\exp(\mathrm{i}\alpha)\Psi(x,y) \qquad \text{with} \qquad \exp(3\mathrm{i}\alpha)=1 \tag{2.6}$$

and $2M+N=n_1$, $M-N=n_2$ have to be integers. Therefore

$$\begin{gathered} M=\tfrac{1}{3}(n_1+n_2) \qquad N=\tfrac{1}{3}(n_1-2n_2) \qquad L=\tfrac{1}{3}(n_2-2n_1) \\ \exp(\mathrm{i}\alpha)=\exp[(2\pi\mathrm{i}/3)(n_1+n_2)]. \end{gathered} \tag{2.7}$$

The wavefunctions are

$$\begin{aligned} \Psi_{n_1,n_2}(\boldsymbol{x})=&\exp\{(2\mathrm{i}\pi/3a)[(n_1+n_2)x+(n_1-2n_2)y]\} \\ &-\exp\{(2\mathrm{i}\pi/3a)[(n_1+n_2)x+(n_2-2n_1)y]\} \\ &+\exp\{(2\mathrm{i}\pi/3a)[(n_2-2n_1)x+(n_1+n_2)y]\} \\ &-\exp\{(2\mathrm{i}\pi/3a)[(n_2-2n_1)x+(n_1-2n_2)y]\} \\ &+\exp\{(2\mathrm{i}\pi/3a)[(n_1-2n_2)x+(n_2-2n_1)y]\} \\ &-\exp\{(2\mathrm{i}\pi/3a)[(n_1-2n_2)x+(n_1+n_2)y]\} \end{aligned} \tag{2.8a}$$

or, introducing the quantities

$$\theta_1=\frac{2\pi}{3a}(2x-y) \qquad \theta_2=\frac{2\pi}{3a}(2y-x) \qquad \theta_3=-\frac{2\pi}{3a}(x+y)$$

such that

$$\theta_1+\theta_2+\theta_3=0 \qquad \theta_3\leqslant\theta_2\leqslant\theta_1\leqslant 2\pi$$

we obtain

$$\Psi_{n_1,n_2}(\theta_1,\theta_2,\theta_3)=\begin{vmatrix}\exp(\mathrm{i}n_1\theta_1) & \exp(\mathrm{i}n_2\theta_1) & \exp[\mathrm{i}(n_1+n_2)\theta_1]\\ \exp(\mathrm{i}n_1\theta_2) & \exp(\mathrm{i}n_2\theta_2) & \exp[\mathrm{i}(n_1+n_2)\theta_2]\\ \exp(\mathrm{i}n_1\theta_3) & \exp(\mathrm{i}n_2\theta_3) & \exp[\mathrm{i}(n_1+n_2)\theta_3]\end{vmatrix} \tag{2.8b}$$

$$\Psi_{n_1,n_2}=-\Psi_{n_2,n_1}=\Psi^*_{n_1,n_1-n_2}=\Psi^*_{-n_1,-n_2}. \tag{2.9}$$

The corresponding energies read

$$E_{n_1,n_2}=\frac{\hbar^2}{2m}\left(\frac{4\pi}{3a}\right)^2(n_1^2+n_2^2-n_1n_2) \qquad n_1>n_2>0. \tag{2.10}$$

The states can be identified in a plot of (n_1+jn_2) as those in the first sector (see figure 1b), with the energy proportional to the squared distance to the origin.

In a similar fashion one could discuss the modes in a triangle with angles $(\pi/2, \pi/3, \pi/6)$ obtained by cutting the equilateral triangle along a mediatrix, and this would exhaust the integrable cases in two dimensions.

In higher dimensions we shall content ourselves with separable problems, although the previous example could be generalised [10]. Equation (2.8b), for instance, exhibits the relationship between wavefunctions in an equilateral triangle and characters of the group SU(3).

3. Arithmetic identities

The identities discussed in this section are all classical [6, 11-14]. We feel nevertheless justified in giving an elementary exposition, related to simple problems in quantum statistics.

Let us start with a one-dimensional gas of non-interacting fermions in a harmonic well with energy levels $\varepsilon_n=\varepsilon_0(2n+1)$. With T the temperature and μ the chemical potential, the partition function is

$$\begin{aligned} z&=\sum\exp[(\mu N-E)/kT]=\prod_{n=0}^{\infty}\sum_{N_n=0,1}\exp\{[\mu-\varepsilon_0(2n+1)]N_n/kT\}\\ &=\prod_{n=0}^{\infty}(1+yq^{2n+1})\end{aligned} \tag{3.1}$$

with the notation

$$y=\exp(\mu/kT) \qquad q=\exp(-\varepsilon_0/kT). \tag{3.2}$$

We assume throughout this section that $|q|<1$, in which case z extends as an entire function in y. When expanding z in a power series in y, each coefficient gives the partition function in the canonical ensemble with a fixed number N of particles

$$z(y;q)=\sum_{N=0}^{\infty}y^N\sum_{0\leqslant n_1<n_2<\ldots<n_N}q^{\sum_{s=1}^{N}(2n_s+1)}. \tag{3.3}$$

The label s is attached to the occupied one-particle levels arranged according to increasing energy. Each configuration of N fermions can be thought of as an excitation on a ground state, where the first N levels are occupied, with minimal energy

$\varepsilon_0 \Sigma_{n=0}^{N-1} (2n+1) = \varepsilon_0 N^2$. This justifies writing $2n_s + 1 = 2s - 1 + 2l_s$; $0 \leqslant l_1 \leqslant l_2 \leqslant \ldots \leqslant l_N$, and

$$z(y;q) = \sum_{N=0}^{\infty} y^N q^{N^2} \sum_{0 \leqslant l_1 \leqslant l_2 \ldots \leqslant l_N} q^{2\Sigma_{s=1}^{N} l_s}.$$

The last sum is readily performed first on l_N, then $l_{N-1}, \ldots$, with the result

$$z(y;q) = \prod_{n=0}^{\infty} (1 + yq^{2n+1}) = 1 + \sum_{N=1}^{\infty} y^N q^{N^2} [(1-q^2)(1-q^4)\ldots(1-q^{2N})]^{-1} \tag{3.4}$$

which is a classical identity due to Euler.

Consider now the same problem with fermions and antifermions of opposite chemical potential, so that the conserved quantity is the number of fermions minus the number of antifermions. The partition function is then obviously (assuming $y \neq 0$)

$$Z(y;q) = z(y;q)z(y^{-1};q) = \prod_{n=0}^{\infty} (1 + yq^{2n+1})(1 + y^{-1}q^{2n+1}). \tag{3.5}$$

We are interested in the (Laurent) expansion

$$Z(y;q) = \sum_{N=-\infty}^{+\infty} y^N Z_N(q). \tag{3.6}$$

Obviously $Z_N(q) = Z_{-N}(q)$, so that it is sufficient to study the case $N \geqslant 0$. As always when dealing with antifermions, it is convenient to introduce negative single-particle energy states. The neutral vacuum, or reference state in Fock space, has all its one-particle negative-energy states occupied. Any Fock state can then be described by enumerating some filled positive-energy states (particles) and holes in the negative-energy sea (antiparticles). In particular, in the sector of positive fermionic charge $N \geqslant 1$, the lowest total energy state implies the occupancy of the first N one-particle states ($E_{\min} = \varepsilon_0 N^2$), and excitations above that level are described in identical terms to those above the ground state. This proves that

$$Z_N(q) = Z_{-N}(q) = q^{N^2} Z_0(q). \tag{3.7}$$

We can relate any neutral excited state to the Fock vacuum by setting a correspondence between one-particle occupied states of decreasing energy (see figure 2). Neutrality and finite total energy of excitation ensure that, far enough down the ladder, the corresponding occupied levels have equal energies, and

$$E = 2\varepsilon_0(r_1 + r_2 + \ldots)$$

with $r_1 \geqslant r_2 \geqslant r_3 \ldots \geqslant 0$. The sum being finite, only a finite number of r are strictly positive. Hence each partition of the integer $E/2\varepsilon_0$ is in one-to-one correspondence with a neutral state of energy E. Denoting by α_k the number of r equal to k, we have

$$Z_0(q) = \prod_{k=1}^{\infty} \sum_{\alpha_k=0}^{\infty} q^{2k\alpha_k} = \prod_{k=1}^{\infty} \frac{1}{1-q^{2k}} \tag{3.8}$$

which is Euler's generating function for partitions. Collecting our results, we find Jacobi's triple product identity in the form

$$\theta(y;q) = yq\theta(yq^2;q) = \sum_{N=-\infty}^{\infty} y^N q^{N^2} = \prod_{k=1}^{\infty} (1-q^{2k})(1+yq^{2k-1})(1+y^{-1}q^{2k-1}). \tag{3.9}$$

We have dropped the subscript 3 in the notation for the elliptic form $\theta(y;q)$.

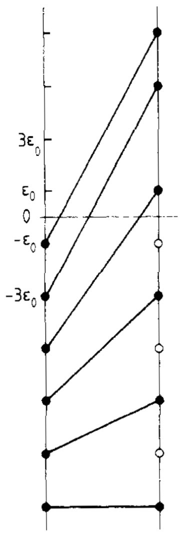


Figure 2. Correspondence between occupied states in the neutral sector, leading to (3.8).

The next step is to introduce, besides fermions and antifermions, bosons and antibosons with equal chemical potentials in absolute value, again in the same harmonic well. The complete partition function is

$$\Xi(y;q)=\frac{Z(y;q)}{Z(-y;q)}=\prod_{k=0}^{\infty}\frac{(1+yq^{2k+1})(1+y^{-1}q^{2k+1})}{(1-yq^{2k+1})(1-y^{-1}q^{2k+1})}=\sum_{n=-\infty}^{\infty}\Xi_N(q)y^N. \tag{3.10}$$

This is a meromorphic function in the complex y plane, with the origin deleted, and the last series is valid for $|q|<|y|<|q|^{-1}$. Furthermore

$$\Xi(q^2y;q)=-\Xi(y;q). \tag{3.11}$$

The integral

$$\left(\oint_{|y|=1}-\oint_{|y|=|q^2|}\right)\frac{\mathrm{d}y}{2\mathrm{i}\pi y^{N+1}}\Xi(y;q)$$

encircles once the simple pole of $\Xi\ (y;q)$ at $y=q$. Cauchy's residue theorem, together with (3.11), yields

$$(1+q^{-2N})\Xi_N(q)=2q^{-N}\prod_{k=1}^{\infty}\left(\frac{1+q^{2k}}{1-q^{2k}}\right)^2$$

and therefore

$$\Xi(y;q)=\prod_{k=1}^{\infty}\frac{(1+yq^{2k-1})(1+y^{-1}q^{2k-1})}{(1-yq^{2k-1})(1-y^{-1}q^{2k-1})}=2\prod_{k=1}^{\infty}\left(\frac{1+q^{2k}}{1-q^{2k}}\right)^2\sum_{N=-\infty}^{\infty}\frac{q^N}{1+q^{2N}}y^N \tag{3.12}$$

an identity again due to Jacobi, valid in the annulus $|q|<|y|<|q|^{-1}$.

We can now make contact with the degeneracy problem. Setting $y=1$ in (3.12), one finds

$$\prod_{k=1}^{\infty}\left(\frac{(1+q^{2k-1})(1-q^{2k})}{(1-q^{2k-1})(1+q^{2k})}\right)^2=1+4\sum_{N=1}^{\infty}\frac{q^N}{1+q^{2N}}. \tag{3.13}$$

The remark, due to Euler, that

$$\prod_{k=1}^{\infty}(1-q^{2k-1})(1+q^k)=\prod_{k=1}^{\infty}\frac{(1-q^{2k-1})(1-q^{2k})(1+q^k)}{(1-q^{2k})}=1 \tag{3.14}$$

allows one to rewrite the left-hand side of (3.13) as

$$\left(\prod_{k=1}^{\infty}(1+q^{2k-1})^2(1-q^{2k})\right)^2$$

which is recognised from identity (3.9) as $\theta(1;q)^2$. Therefore

$$\theta(1;q)^2=\sum_{n_1,n_2=-\infty}^{\infty}q^{n_1^2+n_2^2}=1+4\sum_{N=1}^{\infty}\frac{q^N}{1+q^{2N}}. \tag{3.15}$$

Returning to (3.12), we identify the coefficient of y^0 on both sides of the relation $1=\Xi(y;q^{1/2})\Xi(-y;q^{1/2})$, with the result that

$$1=4\left[\prod_{k=1}^{\infty}\left(\frac{1+q^k}{1-q^k}\right)\right]^4\sum_{N=-\infty}^{\infty}\frac{(-1)^N q^N}{(1+q^N)^2}. \tag{3.16}$$

Making use again of (3.9) and (3.14), we have that

$$\prod_{k=1}^{\infty}\left(\frac{1-q^k}{1+q^k}\right)=\prod_{k=1}^{\infty}(1-q^k)(1-q^{2k-1})=\theta(1,-q).$$

Inserting this in (3.16), and changing q to $-q$, yields

$$\theta(1;q)^4=1+8\sum_{N=1}^{\infty}\frac{q^N}{[1+(-q)^N]^2}.$$

Expanding each denominator on the right-hand side and summing in the opposite order leads to the alternate form

$$\theta(1;q)^4=\sum_{n_1,n_2,n_3,n_4=-\infty}^{\infty}q^{n_1^2+n_2^2+n_3^2+n_4^2}=1+8\sum_{N=1}^{\infty}\left(\frac{Nq^N}{1-q^N}-\frac{4Nq^{4N}}{1-q^{4N}}\right). \tag{3.17}$$

Finally in the study of the equilateral triangle we shall also use the identity

$$\begin{aligned}\Delta(q)&=\theta(1;q)\theta(1;q^3)+q\theta(q;q)\theta(q^3;q^3)\\&=\sum_{n_1,n_2=-\infty}^{\infty}q^{n_1^2+n_2^2-n_1n_2}=1+6\sum_{N=1}^{\infty}\frac{q^N}{1+q^N+q^{2N}}\end{aligned} \tag{3.18}$$

which is equivalent to arithmetic statements on the divisors of $n_1^2+n_2^2-n_1n_2$ [6, 11-14]. A four-dimensional generalisation, analogous to (3.17), is

$$\Delta(q)^2=\sum_{n_1,n_2,n_3,n_4=-\infty}^{\infty}q^{n_1^2+n_2^2+n_3^2+n_4^2-n_1n_2-n_3n_4}=1+12\sum_{N=1}^{\infty}\left(\frac{Nq^N}{1-q^N}-\frac{3Nq^{3N}}{1-q^{3N}}\right). \tag{3.19}$$

A straightforward proof of (3.18) and (3.19) is given in the appendix.

4. Two-dimensional degeneracies

We will study in parallel the spectrum of the square and equilateral triangle, when necessary using as subscripts the symbols □ and △. Our presentation is patterned after the book of Blanchard [15]. Dropping dimensional factors, the energies are given by

$$E_{\square}(n_1, n_2) = n_1^2 + n_2^2 \qquad n_1 > 0, n_2 > 0 \tag{4.1a}$$

$$E_{\triangle}(n_1, n_2) = n_1^2 + n_2^2 - n_1 n_2 \qquad n_1 > n_2 > 0 \tag{4.1b}$$

so that the energies are themselves integers. In the square case, when $n_1 \neq n_2$, the two states (n_1, n_2) and (n_2, n_1) are obviously degenerate. A compilation of the first few levels reveals that many other degeneracies occur. It will be convenient to adopt the following conventions and notations. We will write $\bar{D}(E)$ for the degeneracy (multiplicity) of level E, while $D(E)$ will be equal to $\bar{D}(E)$ if E is not a square, and equal to $\bar{D}(E)+1$ if E is a square. It will be easier to work analytically with $D(E)$ while numerical data will be provided for $\bar{D}(E)$. The distinction will be irrelevant for all asymptotic formulae to be discussed, and the corrections can easily be supplied. A bar on related quantities will similarly mean the replacement of $D(E)$ by $\bar{D}(E)$. By $F(d, E)$ we shall mean

$$F(d, E) = E^{-1} \times [\text{number of values } E' \leqslant E \text{ such that } D(E') = d] \tag{4.2}$$

and we will study the moments

$$\mu_k(E) = \sum_d d^k F(d, E) \qquad k \geqslant 1$$
$$\mu_0(E) = \sum_{d \neq 0} F(d, E). \tag{4.3}$$

The reason for introducing $D(E)$, rather than $\bar{D}(E)$, appears immediately when we expand the right-hand side of (3.15) in a double series. We find

$$\sum_{n=1}^{\infty} q^{n^2} + \sum_{n_1, n_2 = 1}^{\infty} q^{n_1^2 + n_2^2} = \sum_{k=1}^{\infty} \sum_{l=0}^{\infty} (q^{k(1+4l)} - q^{k(3+4l)}). \tag{4.4}$$

The definition of $D(E)$ implies then that it is the coefficient of q^E on both sides and we see that each divisor of E of the form $4l+1$ (respectively $4l+3$) contributes 1 (-1) to $D(E)$. Let us denote generically by p (respectively r) the odd primes of the form $4l+1$ $(4l+3)$. The product of two p or two r is of the form $4l+1$ while the product of a p and a r is of the form $4l+3$. Consequently, if the prime decomposition of $E_{\square}$ is

$$E_{\square} = 2^{\sigma} p_1^{\alpha_1} p_2^{\alpha_2} \ldots r_1^{\beta_1} r_2^{\beta_2} \ldots \qquad p_i \text{ prime} \equiv 1 \pmod 4,\ q_j \text{ prime} \equiv 3 \pmod 4 \tag{4.5}$$

then

$$D_{\square}(E) = \sum_{\substack{0 \leqslant a_i \leqslant \alpha_i \\ 0 \leqslant b_j \leqslant \beta_j}} (-1)^{\Sigma_j b_j} = \prod_i (1+\alpha_i) \prod_j \left(\frac{1+(-1)^{\beta_j}}{2} \right). \tag{4.6}$$

This states that $D_{\square}(E)$ is non-zero only in the case where all β are even, in which case it is given by the number of its odd divisors factorisable into primes $\equiv 1 \pmod 4$, a result which has its roots in the work of Fermat. Conversely from (4.6) one can derive (3.15). Thus the study of the D is a variant of the study of the number of divisors. The formulae and results are quite similar.

Using the same convention in the equilateral triangle case, it follows from (3.18) that (4.6) also holds true, provided we take the p (r) to be primes of the form $3l+1$ $(3l+2)$, and

$$E_{\triangle} = 3^{\sigma} p_1^{\alpha_1} p_2^{\alpha_2} \ldots r_1^{\beta_1} r_2^{\beta_2} \ldots \qquad p_i \text{ prime} \equiv 1 \pmod 3,\ r_j \text{ prime} \equiv 2 \pmod 3. \tag{4.7}$$

In spite of being very explicit, the formula for $D(E)$ is not as informative as one might hope, being related to $\pi(x)$, the number of primes less or equal to x, which behaves for large x as $\mathrm{Li}(x)$ [11, 12]

$$\pi(x) \sim \mathrm{Li}(x) = \int_0^x \frac{\mathrm{d}y}{\ln y} = \frac{x}{\ln(x/\mathrm{e})}[1 + \mathrm{O}((\ln x)^{-2})]. \tag{4.8}$$

If Riemann's hypothesis is true, then the corrections to (4.8) are of the type $\pi(x) - \mathrm{Li}(x) = \mathrm{O}(x^{1/2} \ln x)$. One route to obtain (4.8) is to follow Riemann in studying the function

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_{p \text{ prime}} (1 - p^{-s})^{-1}. \tag{4.9}$$

Both sum and product converge absolutely for $\mathrm{Re}\, s > 1$, and $\zeta(s)$ extends as a meromorphic function in the entire s plane, with a unique simple pole of unit residue at $s = 1$. Similarly in the degeneracy problem we introduce the Dirichlet series [15]

$$\eta_k(s) = \sum_{n=1}^{\infty} \frac{D^k(n)}{n^s} \tag{4.10}$$

for all non-negative integers k, which will allow us to obtain the behaviour of all moments $\mu_k(E)$, defined in (4.3), for large E. Obviously for very small values of E, the explicit expression (4.6) is quite sufficient. The latter enables one to express $\eta_k(s)$ as infinite products over primes:

$$\eta_{k,\square}(s) = \frac{1}{1 - 2^{-s}} \prod_{\substack{p \text{ prime} \\ p \equiv 1 \,(\mathrm{mod}\, 4)}} \frac{P_k(p^{-s})}{(1 - p^{-s})^{k+1}} \prod_{\substack{r \text{ prime} \\ r \equiv 3 \,(\mathrm{mod}\, 4)}} \frac{1}{1 - r^{-2s}} \tag{4.11a}$$

$$\eta_{k,\triangle}(s) = \frac{1}{1 - 3^{-s}} \prod_{\substack{p \text{ prime} \\ p \equiv 1 \,(\mathrm{mod}\, 3)}} \frac{P_k(p^{-s})}{(1 - p^{-s})^{k+1}} \prod_{\substack{r \text{ prime} \\ r \equiv 2 \,(\mathrm{mod}\, 3)}} \frac{1}{1 - r^{-2s}}. \tag{4.11b}$$

These expressions introduce a family of polynomials $P_k(x)$ defined through

$$P_k(x) = (1 - x)^{k+1} \sum_{\alpha=0}^{\infty} (1 + \alpha)^k x^\alpha = (1 - x)^{k+1} \left(\frac{\mathrm{d}}{\mathrm{d}x} x\right)^k \frac{1}{1 - x}. \tag{4.12}$$

P_0 is equal to one, while for $k \geqslant 1$, $P_k(x)$ is a polynomial of degree $k - 1$ with integral coefficients

$$\begin{aligned} &P_k(x) = 1 + [2^k - \tbinom{k+1}{1}]x + [3^k - 2^k\tbinom{k+1}{1} + \tbinom{k+1}{2}]x^2 + \dots \\ &P_k(0) = 1 \qquad P_k(1) = k! \end{aligned} \tag{4.13}$$

The immediate consequences of (4.12) are the relations

$$P_{k+1}(x) = (kx + 1)P_k(x) + x(1 - x)P_k'(x) \tag{4.14a}$$

$$\frac{\mathrm{e}^u}{1 - x\mathrm{e}^u} = \sum_{k=0}^{\infty} \frac{u^k}{k!} \frac{P_k(x)}{(1 - x)^{k+1}} \tag{4.14b}$$

$$\exp[-(k - 1)\theta] P_k(-\exp(2\theta)) = (\cosh\theta)^{k+1} (\mathrm{d}^k/\mathrm{d}\theta^k) \tanh\theta. \tag{4.14c}$$

It follows that $P_k(x)$ is a reciprocal polynomial $[P_k(x) = x^{k-1}P_k(x^{-1})]$ and has its zeros on the negative real axis. A table of the first few P_k is as follows:

$$\begin{aligned} &P_0 = 1 \\ &P_1 = 1 && P_4 = 1 + 11x + 11x^2 + x^3 \\ &P_2 = 1 + x && P_5 = 1 + 26x + 66x^2 + 26x^3 + x^4 \\ &P_3 = 1 + 4x + x^2 && P_6 = 1 + 57x + 302x^2 + 302x^3 + 57x^4 + x^5. \end{aligned} \tag{4.15}$$

To use the Dirichlet series $\eta_k(s)$, obviously analytic for Re s large enough, in the estimate of the moments, one may proceed as follows. First we express $\mu_k(E)$, using a representation of the step function, as

$$\mu_k(E) = \int_{\mathrm{Re}\, s = c} \frac{\mathrm{d\,Im}\, s}{2\pi} E^{s-1} \eta_k(s) \tag{4.16}$$

with c in the analyticity domain. Then we displace the contour to the left until we hit a singularity in $\eta_k(s)$. The latter will occur at $s = 1$, as a pole for $k \geqslant 1$ or a branch point for $k = 0$, as will follow from the representation (4.11). The contribution from this leading singularity will yield the dominant behaviour of $\mu_k(E)$ for large E. Alternatively, and more sloppily, one may observe that a behaviour $\mu_k(E) \sim a(\ln E)^\gamma$ corresponds for $\eta_k(s)$ to a singularity of the type $a\int_1^\infty \mathrm{d}n(\ln n)^\gamma n^{-s} = a\Gamma(\gamma+1)(s-1)^{-\gamma-1}$. Whichever way, we need the rightmost singularity of $\eta_k(s)$.

To illustrate the method consider first $\eta_1(s)$. Then one derives from (4.11)

$$\eta_1(s) = \zeta(s)L(s) \tag{4.17}$$

with

$$L_\square(s) = \prod_{\substack{p\,\mathrm{prime} \\ p \equiv 1\,(\mathrm{mod}\,4)}} \frac{1}{1-p^{-s}} \prod_{\substack{r\,\mathrm{prime} \\ r \equiv 3\,(\mathrm{mod}\,4)}} \frac{1}{1+r^{-s}} = \sum_{n=0}^\infty \frac{(-1)^n}{(2n+1)^s} \tag{4.18a}$$

$$\begin{aligned} L_\triangle(s) &= \prod_{\substack{p\,\mathrm{prime} \\ p \equiv 1\,(\mathrm{mod}\,3)}} \frac{1}{1-p^{-s}} \prod_{\substack{r\,\mathrm{prime} \\ r \equiv 2\,(\mathrm{mod}\,3)}} \frac{1}{1+r^{-s}} \\ &= \sum_{n=0}^\infty \left(\frac{1}{(3n+1)^s} - \frac{1}{(3n+2)^s}\right). \end{aligned} \tag{4.18b}$$

In both cases $L(s)$ is analytic at least for Re $s > 0$, and

$$L_\square(1) = \pi/4 \qquad L_\triangle(1) = \pi/3^{3/2}. \tag{4.19}$$

Consequently $\eta_1(s)$ is meromorphic for Re $s > 0$ with a unique pole at $s = 1$ with known residue. This leads at once to the estimates

$$\mu_{1,\square}(E) \sim \pi/4 \qquad \mu_{1,\triangle}(E) \sim \pi/3^{3/2} \tag{4.20}$$

which of course agree with the Weyl estimate for the leading behaviour of the integrated density of levels. Corrections to (4.20) are available and will be discussed later.

We turn to $\mu_0(E)$, the quantity discussed by Berry [2]. Comparison of $\eta_1(s)$ and $\eta_0(s)$ given by (4.11) yields

$$[\eta_{0,\square}(s)]^2 = \eta_{1,\square}(s)\frac{1}{1-2^{-s}} \prod_{\substack{r\,\text{prime}\\ r\equiv 3(\text{mod}\,4)}} \frac{1}{1-r^{-2s}} \tag{4.21a}$$

$$[\eta_{0,\triangle}(s)]^2 = \eta_{1,\triangle}(s)\frac{1}{1-3^{-s}} \prod_{\substack{r\,\text{prime}\\ r\equiv 2(\text{mod}\,3)}} \frac{1}{1-r^{-2s}}. \tag{4.21b}$$

The products converge to the right of Re $s=\frac{1}{2}$ and hence cannot vanish in this region, so that one can take their square root. From the expression (4.17) we therefore deduce that $\eta_0(s)$ has a branch point at $s=1$. Now we introduce the quantities

$$A_\square = \prod_{r\equiv 3(\text{mod}\,4)} (1-r^{-2}) \qquad A_\triangle = \prod_{r\equiv 2(\text{mod}\,3)} (1-r^{-2}). \tag{4.22}$$

Then

$$\mu_{0,\square}(E) \sim (2A_\square \ln E)^{-1/2} \qquad \mu_{0,\triangle}(E) \sim (2\sqrt{3}\,A_\triangle \ln E)^{-1/2}. \tag{4.23}$$

This means that, far from occupying rather uniformly the integers, the levels are highly degenerate and leave huge unoccupied holes. Asymptotically the probability that an integer belongs to the spectrum is zero!

The corrections to the estimates (4.20) are *a priori* of relative order $(\ln E)^{-1}$, and this will also be true for those pertaining to higher moments. Those arise from the finite terms of $\eta_1(s)$ at $s=1$, once the pole is extracted. This is why we choose $(\ln E)^{-1}$ as the abscissa on figure 3, where we plot $\bar{\mu}_0(E)(\ln E)^{1/2}$ as a function of $(\ln E)^{-1}$ for E up to 10^6. The asymptotic results are marked by arrows.

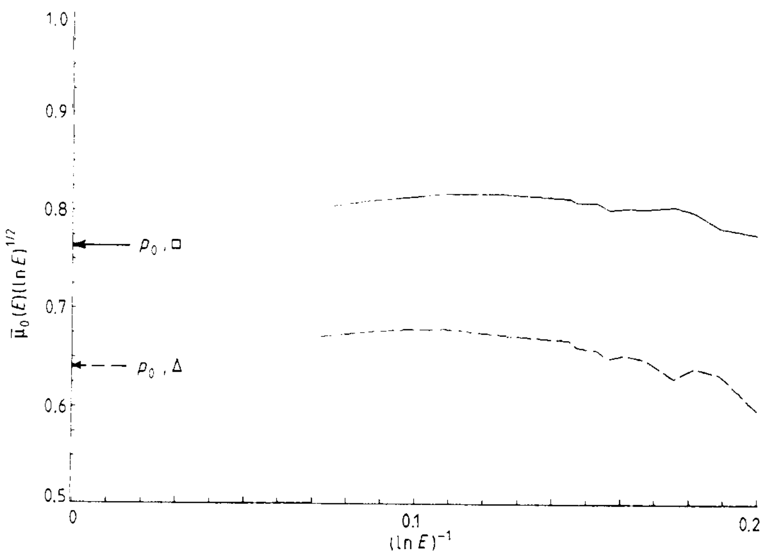


Figure 3. Plot of $\bar{\mu}_0(E)(\ln E)^{1/2}$ against $(\ln E)^{-1}$ for the square (full curve) and the equilateral triangle (broken curve), up to values of E equal to 10^6. The arrows indicate the asymptotic limits (see (4.23)–(4.27)).

For the second moment we note that

$$\eta_{2,\square}(s)=\frac{1}{1+2^{-s}}\zeta^2(s)\zeta(2s)^{-1}L_\square^2(s) \tag{4.24a}$$

$$\eta_{2,\triangle}(s)=\frac{1}{1+3^{-s}}\zeta^2(s)\zeta(2s)^{-1}L_\triangle^2(s) \tag{4.24b}$$

which yield

$$\mu_{2,\square}(E)\sim\tfrac{1}{4}\ln E \qquad \mu_{2,\triangle}(E)\sim\tfrac{1}{6}\ln E. \tag{4.25}$$

It would be interesting to find a shorter derivation of these simple results.

For larger k values it is advantageous to replace the polynomial $P_k(x)$ by

$$Q_k(x)=(1-x)^{2^k-k-1}P_k(x) \tag{4.26}$$

where the prefactor ensures that $Q_k(x)=1+O(x^2)$ around $x=0$. Similar manipulations as above yield

$$\mu_k(E)\sim p_k(\ln E)^{2^{k-1}-1} \qquad (k\geqslant 0) \tag{4.27a}$$

$$p_{k,\square}=\frac{\pi}{4}\left(\frac{\pi A_\square}{8}\right)^{2^{k-1}-1}\frac{1}{\Gamma(2^{k-1})}\prod_{\substack{p\ \text{prime}\\ p\equiv 1\ (\text{mod}\ 4)}}Q_k(p^{-1}) \tag{4.27b}$$

$$p_{k,\triangle}=\frac{\pi}{3^{3/2}}\left(\frac{2\pi}{3^{5/2}}A_\triangle\right)^{2^{k-1}-1}\frac{1}{\Gamma(2^{k-1})}\prod_{\substack{p\ \text{prime}\\ p\equiv 1\ (\text{mod}\ 3)}}Q_k(p^{-1}). \tag{4.27c}$$

The rapid growth of $\mu_k(E)$ in $(\ln E)^{2^{k-1}-1}$ is quite remarkable. We should, of course, insist on the fact that these expressions are valid for k fixed and E going to infinity. Figures 4 and 5 show the convergence of $\bar{\mu}_2(E)(\ln E)^{-1}$ and $\bar{\mu}_3(E)(\ln E)^{-3}$ towards

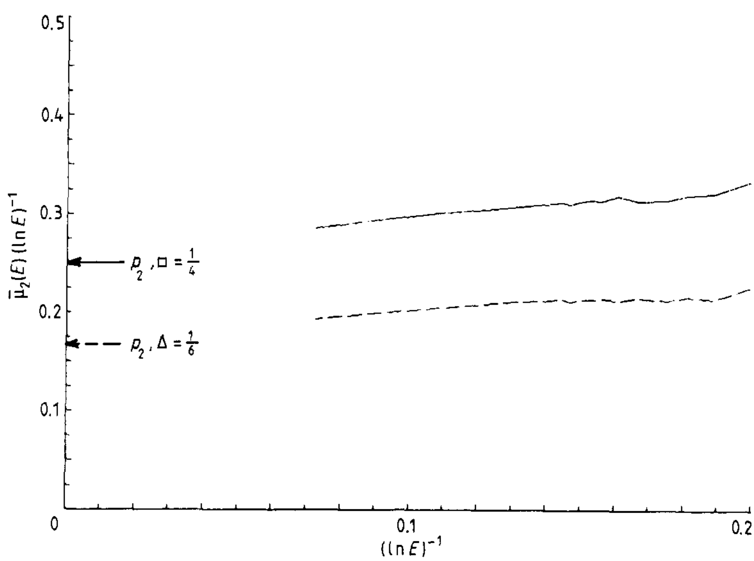


Figure 4. Same as figure 3, for $\bar{\mu}_2(E)(\ln E)^{-1}$

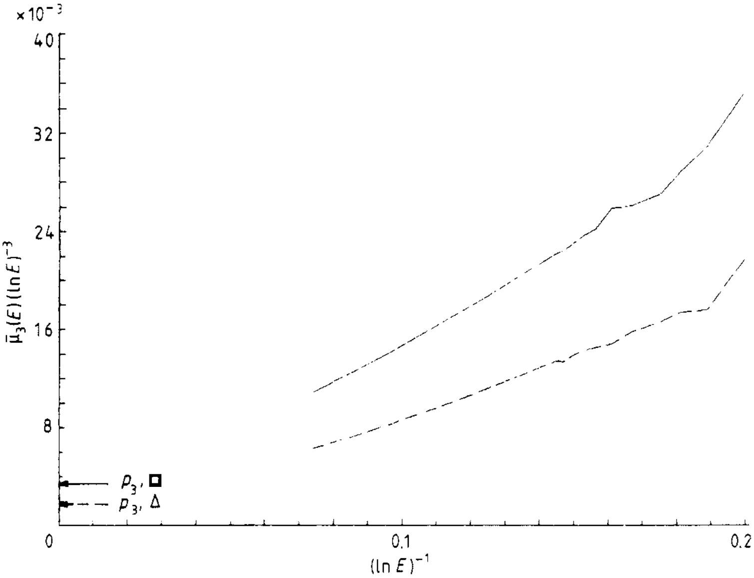


Figure 5. Same as figure 3, for $\bar{\mu}_3(E)(\ln E)^{-3}$.

their limits as functions of $(\ln E)^{-1}$. As k increases $\bar{\mu}_k(E)(\ln E)^{1-2^{k-1}}$ tends to its limit p_k slower and slower.

We recapitulate in the following table the expressions and numerical values of the coefficients p_k in (4.27) up to $k=4$. All products are over primes.

	□	△
p_0	$(2A_\square)^{-1/2}=0.764\,224$	$(2\times 3^{1/2}A_\triangle)^{-1/2}=0{\cdot}638\,909$
p_1	$\pi/4=0.785\,398$	$\pi/3^{3/2}=0.604\,600$
p_2	$1/4=0.250\,000$	$1/6=0.166\,667$
p_3	$\dfrac{\pi^4A_\square^3}{2^{12}\times 3}\prod_{p\equiv 1(\mathrm{mod}\,4)}(1-p^{-1})^4(1+4p^{-1}+p^{-2})$ $=3.3438\times 10^{-3}$	$\dfrac{2^2\pi^4}{3^{10}}A_\triangle^3\prod_{p\equiv 1(\mathrm{mod}\,3)}(1-p^{-1})^4(1+4p^{-1}+p^{-2})$ $=1.8032\times 10^{-3}$
p_4	$\dfrac{\pi^8A_\square^7}{2^{25}7!}\prod_{p\equiv 1(\mathrm{mod}\,4)}(1-p^{-1})^{11}$ $\times(1+11p^{-1}+11p^{-2}+p^{-3})=1.3066\times 10^{-8}$	$\dfrac{2^3\pi^8}{3^{21}\times 5\times 7}A_\triangle^7\prod_{p\equiv 1(\mathrm{mod}\,3)}(1-p^{-1})^{11}$ $\times(1+11p^{-1}+11p^{-2}+p^{-3})=5.405\times 10^{-9}$

We return to (4.2) where all corrections can be supplied explicitly. Define the integrated density of states

$$\begin{aligned} H_\square(E) &= 1+4E\mu_{1,\square}(E)=1+4[E^{1/2}]+4E\bar{\mu}_{1,\square}(E) \\ &= \sum_{n_1,n_2=-\infty}^{\infty}\theta(E-|n|^2)=\pi E+E^{1/4}\Psi_\square(E) \end{aligned} \tag{4.28a}$$

$$\begin{aligned} H_\triangle(E) &= 1+6E\mu_{1,\triangle}(E)=1+6[E^{1/2}]+6E\bar{\mu}_{1,\triangle}(E) \\ &= \sum_{n_1,n_2=-\infty}^{\infty}\theta(E-\|n\|^2)=\frac{2\pi}{3^{1/2}}E+E^{1/4}\Psi_\triangle(E). \end{aligned} \tag{4.28b}$$

The symbol $[E]$ stands for the integer part, and $|n|^2=n_1^2+n_2^2$, $\|n\|^2=n_1^2+n_2^2-n_1n_2$.

The factorisation of $E^{1/4}$ in the correction term is suggested by the following exact expressions, obtained through Poisson's summation formula:

$$H_{\square}(E)=\pi E+E^{1/2}\sum_{(m_1,m_2)\neq(0,0)}\frac{J_1(2\pi|m|E^{1/2})}{|m|} \tag{4.29a}$$

$$H_{\triangle}(E)=\frac{2\pi E}{3^{1/2}}+E^{1/2}\sum_{(m_1,m_2)\neq(0,0)}\frac{J_1((4\pi/3^{1/2})\|m\|E^{1/2})}{\|m\|} \tag{4.29b}$$

where the Bessel function $J_1(z)$ behaves as $(2/\pi z)^{1/2}\sin(z-\pi/4)$ for large z. The functions $\Psi_{\square}(E)$ and $\Psi_{\triangle}(E)$ are represented in figures 6 and 7 for $0\leqslant E\leqslant 300$.

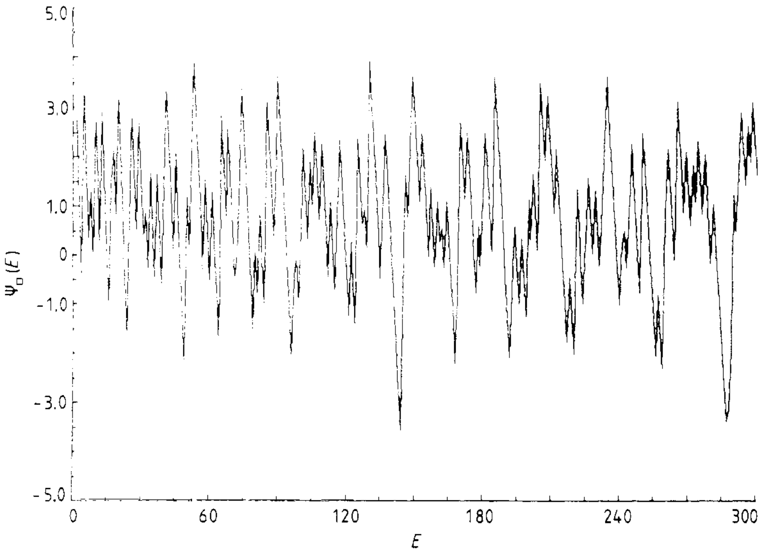


Figure 6. Oscillatory amplitude $\Psi_{\square}(E)$ in the integrated level density of the square, up to $E=300$.

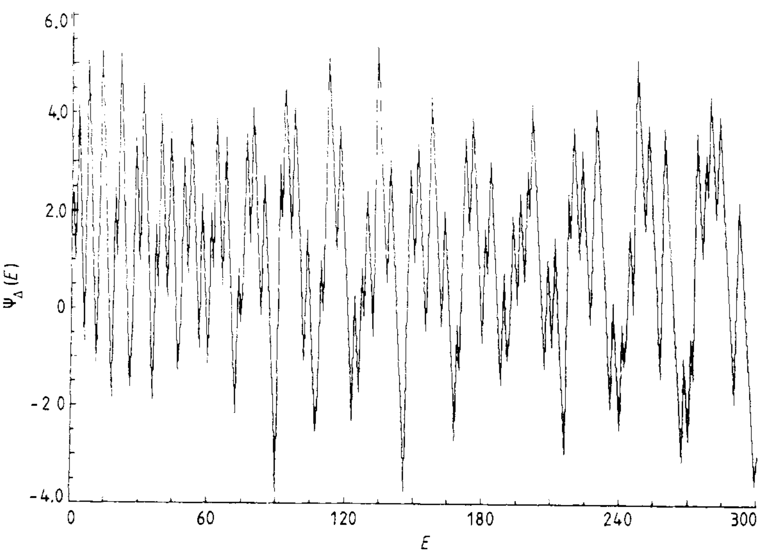


Figure 7. Same as figure 6, for the equilateral triangle.

Note the large oscillations of these functions for values of E as small as a few hundreds. Figure 8 shows a plot of the quantity $-\mathrm{Inf}_{E'\leqslant E}\,\Psi(E')$ against $\ln E$ for $E\leqslant 10^7$ for the square and the triangle, suggesting that $\Psi(E)=\mathrm{O}(\ln E)$. As far as we know, it has not been proven that $\Psi(E)=\mathrm{O}(E^{\delta})$ for every positive δ. The quantity $\mathrm{Sup}_{E'\leqslant E}\,\Psi(E')$ grows much more slowly than $\ln E$; we shall not discuss it here.

To close this section we examine two other aspects of the distribution of degeneracies, $F(d, E)$, namely its behaviour at fixed d, when E gets large, and the maximal degeneracy $D_{\max}(E)$ of those energy levels smaller than or equal to E. To illustrate the first point consider $F(2, E)$. To estimate this quantity, for instance in the square case, define $\omega(n)=1$ if $D(n)=2$ and 0 otherwise, then

$$\sum_{n=1}^{\infty}\frac{\omega_{\square}(n)}{n^s}=\frac{1}{1-2^{-s}}\Bigg(\sum_{\substack{p\,\text{prime}\\ p\equiv 1(\mathrm{mod}\,4)}} p^{-s}\Bigg)\prod_{\substack{r\,\text{prime}\\ r\equiv 3(\mathrm{mod}\,4)}}\frac{1}{1-r^{-2s}}. \tag{4.30}$$

According to (4.8) the number of primes up to x is asymptotically $x/\ln(x/e)$. Since those which have a residue $1(\mathrm{mod}\,4)$ constitute asymptotically half of them [16], then

$$\sum_{\substack{p\,\text{prime}\\ p\equiv 1(\mathrm{mod}\,4)}} p^{-s}\sim\tfrac{1}{2}\int_{\mathrm{est}}^{\infty}\frac{\mathrm{d}x}{\ln x}\,x^{-s}\sim-\tfrac{1}{2}\ln(s-1). \tag{4.31}$$

Consequently

$$F_{\square}(2, E)=\frac{1}{E}\sum_{n\leqslant E}\omega_{\square}(n)\sim(A_{\square}\ln E)^{-1}=1.168\,07\,(\ln E)^{-1}. \tag{4.32a}$$

Using a similar property of primes $\equiv 1(\mathrm{mod}\,3)$, we obtain

$$F_{\triangle}(2, E)=\frac{1}{E}\sum_{n\leqslant E}\omega_{\triangle}(n)\sim\tfrac{3}{4}(A_{\triangle}\ln E)^{-1}=1.060\,54\,(\ln E)^{-1}. \tag{4.32b}$$

For larger even values of d one can also show that $F(d, E)$ behaves as

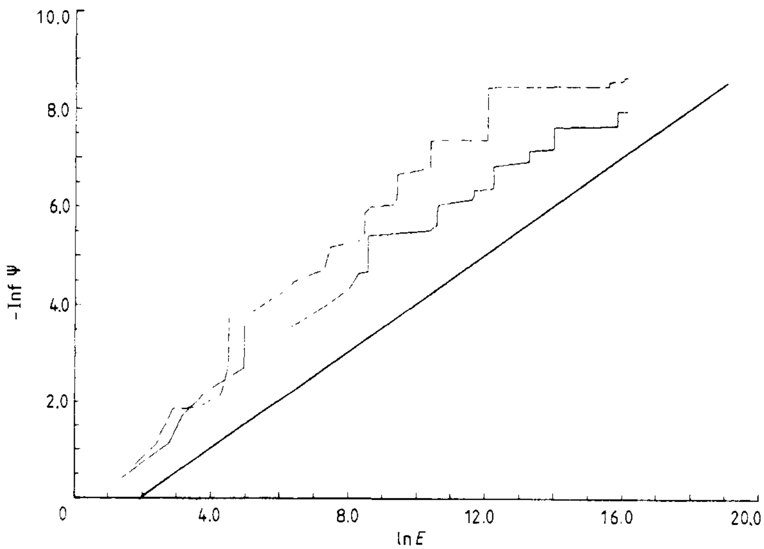


Figure 8. Plot of $-\mathrm{Inf}\,\Psi(E)$ as function of $\ln E$, for E up to 10^7. The full curve refers to the square, the broken curve to the equilateral triangle. The straight line with slope $\frac{1}{2}$ is a guide for the eye.

$(\ln E)^{-1}(\ln(\ln E))^{\delta(d)}$, where $\delta(d)$ is a positive, d-dependent integer: $\delta(2)=0$, $\delta(4)=1,\ldots$. On the other hand, $F(d, E)$ decreases much faster, like $E^{-1/2}$, for odd d, since odd degeneracies occur only for values of E which are squares, as follows from (4.6).

These estimates suggest that the most likely degeneracy up to some value E, i.e. the value of d which maximises $F(d, E)$, grows to infinity extremely slowly. For instance, up to $E = 10^6$, the most likely degeneracy is still 2. This value $d = 2$ is obtained 103 326 times for the square and 94 885 times for the triangle, for $1 \leq E \leq 10^6$. On the other hand, $d = 0$, i.e. absence of level, occurs respectively 784 092 and 819 600 times in the same range.

Finally we turn to an evaluation of the largest degeneracy $D_{\max}(E) = \mathrm{Sup}_{1\leq E'\leq E}\, D(E')$ occurring in the range 1 to E. From (4.6) it is reasonable to assume that the values of E generating the largest degeneracies are of the form $E_q = 5\times 13\times\ldots p_q$, i.e. the products of the first q primes $\equiv 1 (\mathrm{mod}\, 4)$ in the square case, or $E_q = 7\times 13\times\ldots p_q$, i.e. the first q primes $\equiv 1(\mathrm{mod}\, 3)$ in the equilateral case. The corresponding degeneracy is 2^q with

$$q \sim \tfrac{1}{2}p_q/\ln(p_q/\mathrm{e}) \tag{4.33}$$

(using again the fact that asymptotically half the primes belong to these congruences). Then

$$E_q \sim \frac{1}{2}\int^{p_q} \frac{\mathrm{d}p}{\ln p}\ln p \sim \tfrac{1}{2}p_q + C \tag{4.34}$$

and

$$\ln D_{\max}(E) \sim \frac{\ln 2}{\ln((2/e)\ln E)}(\ln E - C) \tag{4.35}$$

with a certain constant C. Hardy and Wright [11] give a rigorous version of this argument in the similar case of the divisors, which leads to an identical result. Numerical data shown on figure 9 are in excellent agreement with (4.35). We plot $\ln \bar{D}_{\max}(E)\ln((2/e)\ln E)$ against $\ln E$ for $E \leq 2\times 10^7$. The straight line has slope ln 2.

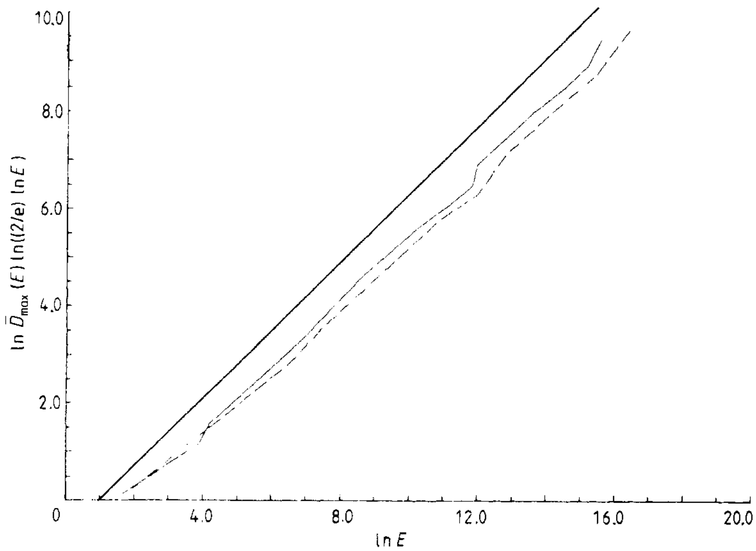


Figure 9. Plot of $\ln \bar{D}_{\max}(E)\ln((2/e)\ln E)$ against $\ln E$ for E up to 2×10^7. Full curve: square; broken curve: equilateral triangle. The straight line has slope ln 2 (see (4.35)).

5. Examples in three and four dimensions

In a cube, the energy levels, in units $\hbar^2\pi^2/2ma^2$, are given by

$$E=(n_1^2+n_2^2+n_3^2) \qquad n_1,\ n_2,\ n_3 \text{ positive integers.} \tag{5.1}$$

The number of levels up to E grows like $E^{3/2}$. More precisely the function

$$H(E)=\sum_{n_1,n_2,n_3=-\infty}^{\infty}\theta(E-n_1^2-n_2^2-n_3^2)=8\bar{H}_3(E)+12\bar{H}_2(E)+6\bar{H}_1(E)+1 \tag{5.2}$$

counts 8 times the three-dimensional levels, adds 12 times those of the corresponding square box, 6 times the one-dimensional spectrum and finally adds unity. In § 4, we discussed $\bar{H}_2$ which behaves as E, and of course $H_1(E)=[E^{1/2}]$. We have

$$H(E)=\frac{4\pi}{3}E^{3/2}+\sum_{(m_1,m_2,m_3)\neq(0,0,0)}\varphi_{m_1m_2m_3}(E)$$

with (5.3)

$$\varphi_{m_1m_2m_3}(E)=\frac{E^{1/2}}{\pi|m|^2}\left(\frac{\sin(2\pi|m|E^{1/2})}{2\pi|m|E^{1/2}}-\cos(2\pi|m|E^{1/2})\right)$$

and $|m|^2=m_1^2+m_2^2+m_3^2$.

As before, we study the moments of the degeneracy distribution

$$\bar{\mu}_k(E)=\frac{1}{E}\sum_{n\leqslant E}\bar{D}^k(n)=\sum_{d=0}^{\infty}d^k\bar{F}(d,E) \tag{5.4}$$

where $\bar{D}$ again refers to the true Dirichlet problem, while D will admit the possibility that some of the n_i in (5.1) vanish. The difference is immaterial for the asymptotic properties. Equation (5.3) contains the estimate

$$\mu_1(E)\sim\bar{\mu}_1(E)\sim\tfrac{1}{6}\pi E^{1/2} \tag{5.5}$$

and suggests that

$$H(E)-\tfrac{4}{3}\pi E^{3/2}=\mathrm{O}(E^{1/2}).$$

Arithmetical properties on sums of three squares are not easily accessible except for the following result, due to Gauss and Eisenstein [11, 12], that the complementary of the spectrum is described as

$$D(n)=0\Leftrightarrow n=4^a(8b+7) \qquad a,b\geqslant 0. \tag{5.6}$$

As a consequence $F(0,E)$ has a non-zero limit as $E\to\infty$

$$F(0)=\lim_{E\to\infty}F(0,E)=\tfrac{1}{8}\sum_{a=0}^{\infty}4^{-a}=\tfrac{1}{6} \tag{5.7}$$

obtained by setting successively $a=0,1,2,\ldots$, in (5.6). In other words, the spectrum only occupies $\frac{5}{6}$ of the integers.

Except perhaps for finer details, the distribution of degeneracies investigated numerically seems well described by the statement that (5.5) gives the unique scale for large E, in contradistinction with the two-dimensional cases. We conjecture that

$$\mu_k(E)\sim c_k\mu_1(E)^k \tag{5.8}$$

and we speculate that one can find a limiting distribution function $K(x)$

$$K(x) = \lim_{E\to\infty} \sum_{d \le \frac{1}{6}\pi E^{1/2} x} F(d, E)$$
$$K(0) = F(0) = \tfrac{1}{6} \qquad K(\infty) = 1. \tag{5.9}$$

We insist on the speculative character of (5.9) which, if true, would yield the coefficients c_k in (5.8) as moments of $\mathrm{d}K(x)$. From the data we obtained the plot of figure 10. In particular the value at the origin agrees satisfactorily with the prediction (5.7). It would be desirable to find an analytic expression for the scaling function $K(x)$. The data suggest a peak in the derivative $\mathrm{d}K/\mathrm{d}x$ at some value of x around the expectation $\langle x\rangle = c_1 = 1$.

One could now study other integrable systems in three dimensions. Coxeter [7] classifies three irreducible simplices, all derived from the cube, which are likely to exhibit similar properties as those described above.

We have chosen to compare them with another commensurate reducible case obtained by choosing appropriately the sides in a *rectangular* prism with base an equilateral triangle (ratio of height to base side $= \frac{3}{4}$), as shown in figure 11. If a is the height, and in units of $\hbar^2\pi^2/2ma^2$, the energies are given by

$$E = n_1^2 + n_2^2 - n_1 n_2 + n_3^2 \qquad n_2 > n_1 > 0, \qquad n_3 > 0. \tag{5.10}$$

It is readily found that

$$\mu_1(E) \sim \frac{2\pi}{9\sqrt{3}} E^{1/2} \tag{5.11}$$

and the ratio of this value to the one pertaining to the cube is the ratio of their volumes $= 4 \times 3^{-3/2}$. Again there exists asymptotically a finite fraction of integers not belonging to the spectrum. We have

$$n = 9^a(9b+6) \Rightarrow D(n) = 0. \tag{5.12}$$

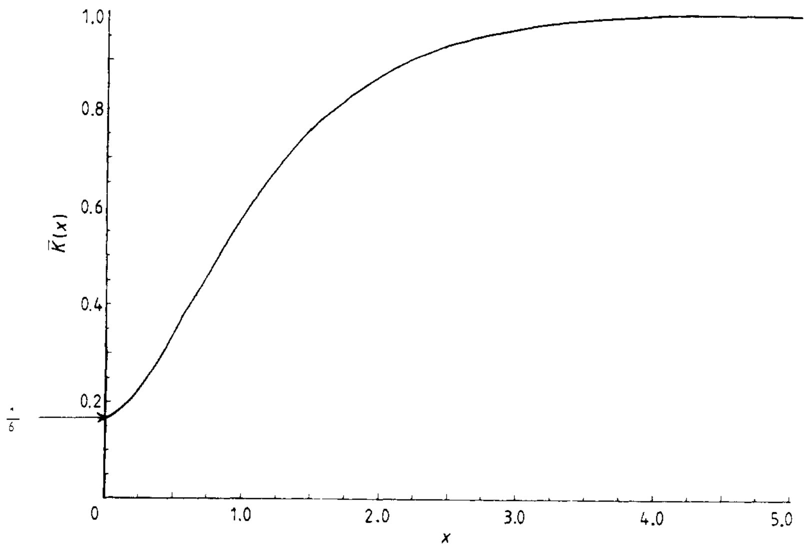


Figure 10. Scaling function $\bar{K}(x) = K(x)$ for the degeneracies of levels in the cube, defined in (5.9). Note the value $K(0) = \frac{1}{6}$.

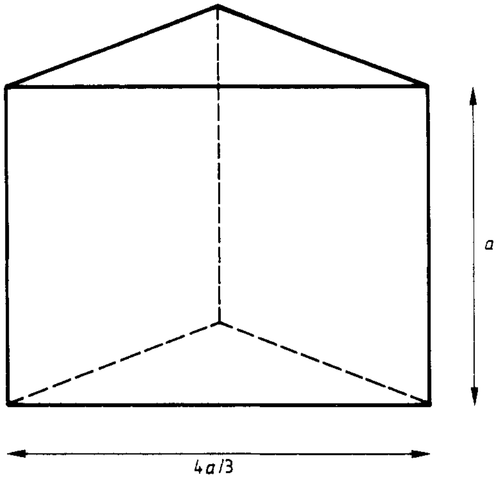


Figure 11. Rectangular prism leading to an integrable commensurate system.

Modulo 9, n_3^2 takes the values 0, 1, 3, 4 and 7, while $n_1^2+n_2^2-n_1n_2$ takes the values 0, 1, 4 and 7. Upon addition all numbers but 6 are represented. If now $n\equiv 0 \pmod 9$ belongs to the spectrum, by enumeration it is seen that both n_3^2 and $n_1^2+n_2^2-n_1n_2$ are zero $\pmod 9$; hence $n_3\equiv 0 \pmod 3$ and $n_1\equiv n_2\equiv 0, \pm 3 \pmod 9$, so that n_1 and n_2 are also divisible by 3. We can therefore repeat the argument with $n_1/3$, $n_2/3$, $n_3/3$ until the energy has no divisor equal to 9, in which case its residue mod 9 is a number different from 0 and 6. This proves (5.12). As a consequence, in the limit $E\to\infty$, there exists a finite probability $F(0)$ for an integer not to belong to the spectrum, and according to (5.12) it is greater than or equal to $\frac{1}{9}\Sigma_0^\infty 1/9^a=\frac{1}{8}$:

$$\lim \operatorname{Inf} \bar{F}(0, E) \geqslant \tfrac{1}{8}. \tag{5.13}$$

We suspect that $\lim_{E\to\infty} \bar{F}(0, E)=\bar{F}(0)$ is equal to $\frac{1}{8}$. Figure 12 is a plot of $F(0, E)$ as a function of E^{-1}, comparing the behaviour for the cube (full curve) and the prism (broken curve), with the limits $\frac{1}{6}$ and $\frac{1}{8}$ shown by arrows. A scaling function, analogous to $K(x)$ introduced in (5.9) for the cube, can also be conjectured for the prism, up to a change in the numerical coefficient to normalise the first moment to unity. We postpone a discussion of the maximal degeneracy to the end of this season.

In a four-dimensional hypercube, the levels are sums of four squares

$$E=n_1^2+n_2^2+n_3^2+n_4^2 \qquad n_i>0. \tag{5.14}$$

As before, $\bar{D}(E)$ denotes the degeneracy, while $16D(E)$ will stand for the coefficient of q^E $(E\geqslant 1)$ on the right-hand side of equation (3.17): $D(n)$ is half the sum of the divisors of n which are not multiples of 4[$d|n$ or $d\nmid n$ stands for d does or does not divide n]

$$D(n)=\tfrac{1}{2}\sum_{\substack{d|n\\ 4\nmid d}} d. \tag{5.15}$$

The difference between $D(n)$ and $\bar{D}(n)$, which affects only boundary subdominant terms, can be made explicit by splitting appropriately the quadruple sum $\Sigma_{-\infty}^{\infty} q^{n_1^2+n_2^2+n_3^2+n_4^2}$. The quantity $D(n)$ is closely related to the classical function $\sigma(n)$,

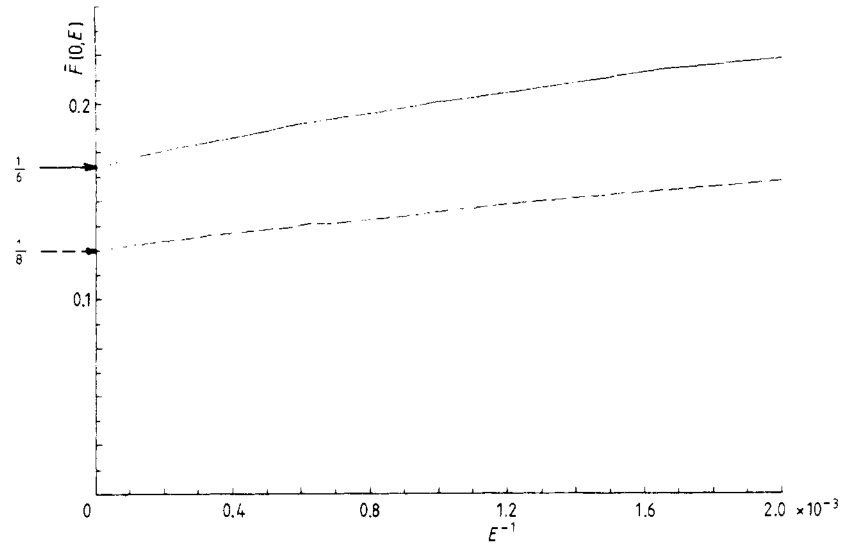


Figure 12. Plot of $\bar{F}(0, E)$ against E^{-1} for the cube (full curve) and the prism (broken curve); the arrows indicate the respective limits $\frac{1}{6}$ and $\frac{1}{8}$ (the latter being only a conjecture).

the sums of divisors of n (1 and n included)

$$\sigma(n) = \sum_{d|n} d \tag{5.16}$$

and of course the treatment of both is closely parallel. If n is factorised over primes as

$$n = 2^{\sigma} \prod_{p \text{ odd prime}} p^{\alpha} \tag{5.17}$$

then

$$D(n) = \tfrac{1}{2}(3 - 2\delta_{\sigma,0}) \prod_{p \text{ odd prime}} \frac{p^{\alpha+1} - 1}{p - 1}. \tag{5.18}$$

Hence

$$\begin{aligned}\eta_1(s) = \sum_{n=1}^{\infty} \frac{D(n)}{n^s} &= \frac{1}{2} \frac{1 + 2^{1-s}}{1 - 2^{-s}} \prod_{p \text{ odd prime}} \left(\frac{1}{1 - p^{1-s}} \frac{1}{1 - p^{-s}} \right) \\ &= \tfrac{1}{2}(1 - 2^{2-2s})\zeta(s)\zeta(s-1).\end{aligned} \tag{5.19}$$

This function has a leading singularity (a pole) at $s = 2$, with a residue equal to $3\zeta(2)/8 = \pi^2/16$. Using similar arguments as in the previous section, we deduce that the first moment $\mu_1(E)$ is given by

$$\mu_1(E) \sim (\pi^2/32)E \tag{5.20}$$

which is of course an asymptotic estimate for $1/16E$ times the number of points with integral coordinates inside a sphere of radius $\sqrt{E}$ in four dimensions. The Fermat–Lagrange theorem asserts that every integer can be written as a sum of four squares, which translates into

$$\mu_0(E) \to 1. \tag{5.21}$$

From (5.18) we can also estimate the second and higher moments. For instance we find for $\eta_2(s)$

$$\eta_2(s)=\sum_1^\infty \frac{D^2(n)}{n^s}=\tfrac{1}{4}\left(1+9\sum_{\sigma=1}^{\infty}2^{-\sigma s}\right)\prod_{p\,\text{odd prime}}\sum_{\alpha=0}^{\infty}\left(\frac{p^{\alpha+1}-1}{p-1}\right)^2 p^{-\alpha s}$$
$$=\frac{1}{4}\frac{1+2^{3-s}}{1-2^{-s}}\prod_{\substack{p\,\text{odd}\\ \text{prime}}}\frac{1+p^{1-s}}{(1-p^{2-s})(1-p^{1-s})(1-p^{-s})}$$
$$=\frac{1}{4}\frac{(1+2^{3-s})(1-2^{2-s})(1-2^{1-s})}{1+2^{1-s}}\frac{\zeta(s-2)\zeta^2(s-1)\zeta(s)}{\zeta(2s-2)}. \tag{5.22}$$

The leading singularity is a simple pole at $s=3$ with a residue $\frac{3}{8}\zeta(3)$. Hence

$$\mu_2(E)\sim\frac{\zeta(3)}{8}E^2=0.150\,257\,113\,E^2. \tag{5.23}$$

Higher order series will introduce new polynomials, as in the two-dimensional case. We quote the result for $\eta_3(s)$:

$$\eta_3(s)=\sum_1^\infty\frac{D^3(n)}{n^s}$$
$$=\frac{1}{8}\frac{(1+13\times2^{1-s})(1-2^{3-s})(1-2^{2-s})(1-2^{1-s})}{(1+3\times2^{2-s}+2^{3-2s})}$$
$$\times\prod_{p\,\text{prime}}[1+2p^{2-s}(1+p^{-1})+p^{3-2s}]\zeta(s-3)\zeta(s-2)\zeta(s-1)\zeta(s) \tag{5.24}$$

leading to

$$\mu_3(E)\sim\frac{147}{9728}\left(\prod_{p\,\text{prime}}(1+2p^{-2}+2p^{-3}+p^{-5})\right)\zeta(2)\zeta(3)\zeta(4)\,E^3 \tag{5.25}$$
$$\sim 0{\cdot}091\,712\,E^3.$$

Very much as in the three-dimensional case, $\mu_1(E)$ defines the only scale, and it can be easily proven that

$$\mu_k(E)\sim c_k\mu_1(E)^k. \tag{5.26}$$

In particular

$$\mu_2(E)/\mu_1^2(E)\to1.579\,56=c_2\qquad \mu_3(E)/\mu_1^3(E)\to3.1259=c_3.$$

All these limiting ratios are exactly computable. A scaling function $K(x)$, shown in figure 13, and defined in analogy with (5.9)

$$K(x)=\lim_{E\to\infty}\sum_{d\leqslant(\pi^2/32)Ex}F(d,E) \tag{5.27}$$

has c_k for moments

$$c_k=\lim_{E\to\infty}\frac{\mu_k(E)}{(\mu_1(E))^k}=\int_0^\infty x^k\,\mathrm{d}K(x). \tag{5.28}$$

We have only shown here that the left-hand side exists in four dimensions. But we conjecture that the existence of a limit law $K(x)$ is general for integrable systems of the type discussed in this paper, in any dimension larger than two.

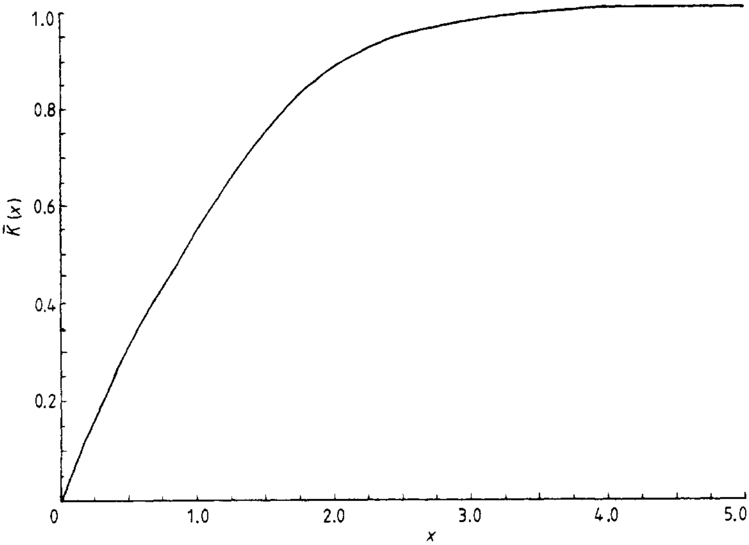


Figure 13. Scaling function $\bar{K}(x)$ for the distribution of degeneracies in the four-dimensional hypercube (see (5.27)).

Finally we come to the discussion of the largest degeneracy encountered up to E: $D_{\max}(E)$. For the four-dimensional hypercube we observe that $D(n) \leqslant \frac{1}{2}\sigma(n)$, with equality if and only if n is not $\equiv 0 (\bmod 4)$. For $\sigma(n)$ one can show [11] that

$$\lim \operatorname{Sup} \frac{\sigma(n)}{n \ln(\ln n)} = e^{\gamma} \tag{5.29}$$

where γ is Euler's constant. Thus in our case it is likely that

$$D_{\max}(E)/E \sim \tfrac{1}{2} e^{\gamma} \ln(\ln E) \qquad (4\text{D}) \tag{5.30}$$

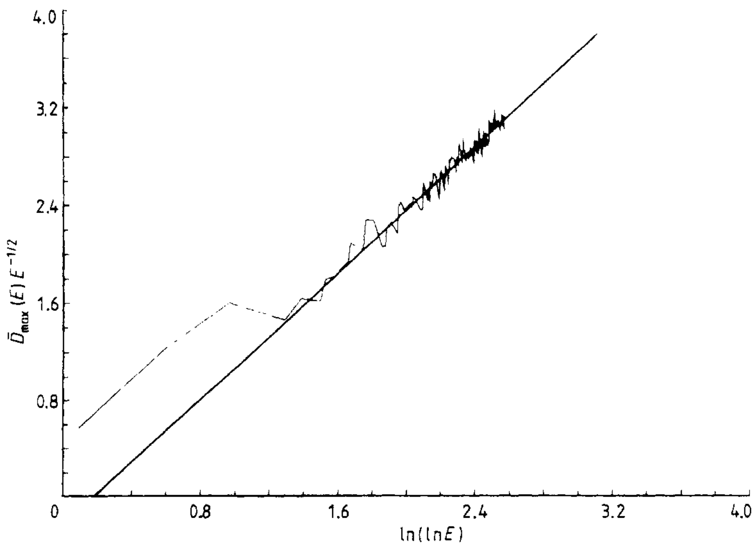


Figure 14. Plot of $\bar{D}_{\max}(E)\, E^{-1/2}$ against $\ln(\ln E)$ for the levels in a cube. The straight line has a slope $a = 1.30$.

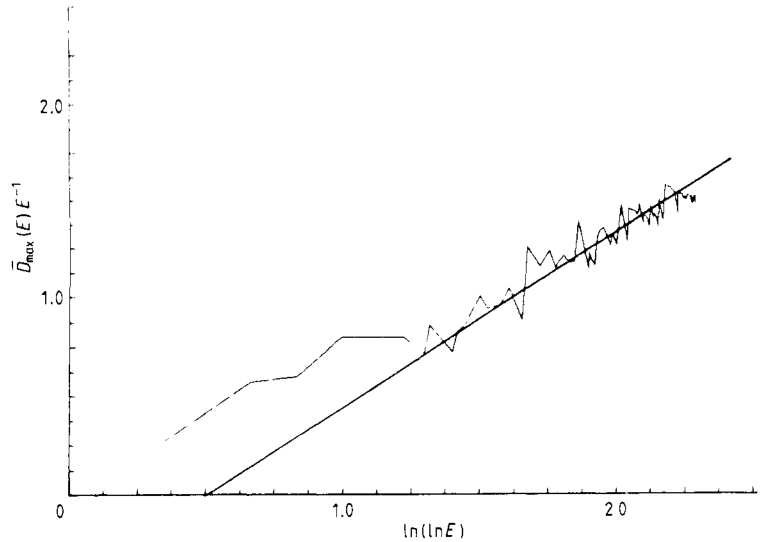


Figure 15. Plot of $\bar{D}_{max}(E)E^{-1}$ against ln(ln E) for the levels in a four-dimensional hypercube. The straight line has a slope $\frac{1}{2}e^{\gamma}$ (see (5.30)), γ being Euler's constant.

which shows that $D_{max}(E)$ grows slightly faster than the *natural* scale $\mu_1(E)\sim(\pi^2/32)E$.

This suggests the conjecture that, in any dimension larger than two, the ratio $D_{max}(E)/\mu_1(E)$ behaves as ln(ln E), and for instance that in three dimensions

$$D_{max}(E)E^{-1/2}\sim a\ln(\ln E) \qquad (3\text{D}). \tag{5.31}$$

Figures 14 and 15 show respectively the quantities $\bar{D}_{max}(E)E^{-1/2}$ for the cube and $\bar{D}_{max}(E)E^{-1}$ for the hypercube, as functions of ln(ln E). The two curves look very similar. The straight line in figure 15 has the slope of (5.30): $\frac{1}{2}e^{\gamma}$, while in figure 14 we have a rough measurement $a = 1.30$, which we are unable to obtain analytically.

What has been said in the case of the hypercube could be repeated in the case of a four-dimensional box equal to the cartesian product of equal equilateral triangles in two orthogonal 2-planes. The reasoning would be based on (3.19) for the generating function $\Delta^2(q)$. In particular the Fermat–Lagrange theorem also holds in this case.

6. Concluding remarks

We have certainly not exhausted the subject of 'accidental' degeneracies (this is really a misnomer) in simple integrable systems. On the mathematical side, a large amount of results and guesses need clarification, although some might be discussed in the literature. One could systematically go through the list of dimensions and fundamental domains. We did not investigate systems in dimensions greater than four: could it be that the scaling functions $K(x)$ assume a simple form as $d\to\infty$? Odd dimensions offer notorious mathematical difficulties. It would also certainly be desirable to offer 'simple' derivations of some of the relevant arithmetic identities, as was initiated in § 3.

We have observed that certain regularities are present. Clearly two is a 'lower critical dimension' with interesting 'sparsity' effects, and four is an upper one. In three dimensions, a finite fraction of the integers is not represented in the spectrum, this fraction being given by a simple rational expression.

Unfortunately we did not answer the question of characterising 'physically' the degeneracies in terms of some hidden invariance. The only simple remark is that one can ascertain *a priori* that, for every level E, we also have a level n^2E for every integer n, since we can fit in the boxes that we consider boxes of size reduced by n and extend a wavefunction in any one of them by reflections in the original one. Other results, such as (4.25), also suggest an underlying simple explanation.

Are these degeneracies, and some of their curious properties, particularly in two dimensions, physically observable? One could, for instance, think of a peculiar sensitivity to random perturbations. Take the case of a localised perturbation around a point x_0 with intensity λ. To lowest order, among D degenerate levels, one is displaced by an amount $\delta E = \Sigma_{a=1}^{D} |\varphi_a(x_0)|^2$, where $\varphi_a(x)$ runs over an orthonormal basis of wavefunctions in the degenerate subspace. As x_0 describes the domain B, the quantity δE fluctuates around its mean value $\langle \delta E \rangle = \lambda D/V$ where V is the volume of B. The proportionality to D is a sign that large degeneracies will enhance the sensitivity to small perturbations.

Another question, which is related to the previous one, is to ask for a remnant of such clusterings in the spectrum of slightly deformed systems.

In any case, it is of some value to be aware of the amount of order and chaos in the most elementary spectra, if only to be able to evaluate the distinction with non-integrable systems. It would be of great interest in this respect to get a handle on those of the family of pseudo-integrable billiards discussed by Berry and his collaborators.

Acknowledgment

We are grateful to Michel Gaudin for some interesting discussions.

Appendix

Our aim is to give a derivation of (3.18) and (3.19). The left-hand side of (3.18) reads

$$\Delta(q) = \sum_{m,n} q^{m^2+n^2+mn} = \sum_{n_1+n_2+n_3=0} q^{(n_1^2+n_2^2+n_3^2-n_1n_2-n_2n_3-n_3n_1)/3} \tag{A1}$$

where the quadratic form in integers gives the square modulus of $(m+jn)$, $j = \exp(2i\pi/3)$, i.e. the squared distance to the origin of the points of an equilateral triangular lattice.

It is well known that a three-dimensional cubic lattice has, perpendicular to the direction (111), a sequence of planes $ABCABC\ldots$ where A is a triangular lattice and B and C, projected on the plane $x+y+z=0$, are respectively the centres of up or down triangles. This suggests that we introduce, besides $\Delta(q)$, the quantity

$$\Delta_1(q) = \sum_{n_1+n_2+n_3=1} q^{(n_1^2+n_2^2+n_3^2-n_1n_2-n_2n_3-n_3n_1)/3}. \tag{A2}$$

The analogous quantity $\Delta_{-1}(q)$, which would correspond to the plane $n_1+n_2+n_3=-1$, is equal to $\Delta_1(q)$. Also $\Delta_1(q)$ is only well defined once a choice of a cubic root of q

has been made. This will be implied in the following. We can therefore write the following identity

$$\theta^3(y;q) = \sum_{n_1,n_2,n_3} y^{n_1+n_2+n_3} q^{n_1^2+n_2^2+n_3^2}$$

$$= \Delta(q^2) \sum_{p=-\infty}^{\infty} y^{3p} q^{3p^2} + \Delta_1(q^2) \sum_{p=-\infty}^{\infty} (y^{3p+1} q^{(3p+1)^2/3} + y^{3p+2} q^{(3p+2)^2/3})$$

$$= \Delta(q^2)\theta(y^3;q^3) + \Delta_1(q^2) q^{1/3} [y\theta(y^3q^2;q^3) + y^2 q\theta(y^3q^4;q^3)]. \tag{A3}$$

This readily follows by slicing the cubic lattice in planes $ABCABC\ldots$ and expressing the squared distance to the origin as the sum of squared distances from the origin to its projection in the plane and from this projection to the lattice point in the plane. As a consequence, the Laurent series for

$$F(y;q) = \theta(-y;q)^3/\theta(-y^3;q^3) \tag{A4}$$

will only have $\Delta(q^2)$ as a term of degree zero in y, since the remaining two terms are respectively multiplied by j and j^2 when y is changed into jy. It reads

$$F(y;q) = \Delta(q^2) + \sum_{n=1}^{\infty} F_n(q)[y^n + y^{-n}] \tag{A5}$$

and converges for $|q| < |y| < |q|^{-1}$. We compute the coefficients $F_n(q)$ using the same technique as in § 3, namely Cauchy's theorem, based on the fact that $F(yq^2;q) = F(y;q)$, which follows from (3.9), the key identity. In the ring $|q|^2 \leqslant |y| \leqslant 1$, F has two simple poles at $y = jq$ and j^2q and a double zero at $y = q$. Since $\theta(-j^2q;q) = \theta(-(1/jq)q^2;q) = -j\theta(-1/jq;q) = -j\theta(-jq;q)$, we have $\theta(-j^2q;q)^3 = -\theta(-jq;q)^3$; hence

$$(1-q^{-2n})F_n(q) = \frac{\theta(-jq;q)^3}{3\prod_{n=1}^{\infty}(1-q^{6n})^3}\frac{1}{q^n}(j^{2n}-j^n) \qquad n \neq 0. \tag{A6}$$

From (3.9) again

$$\theta(-jq;q) = (1-j^2)\prod_{n=1}^{\infty}(1-q^{2n})(1-jq^{2n})(1-j^2q^{2n}) = (1-j^2)\prod_{n=1}^{\infty}(1-q^{6n}). \tag{A7}$$

Also

$$j^{2n} - j^n = (j^2 - j) \times \begin{cases} 0 \text{ if } n \equiv 0 \pmod 3 \\ 1 \text{ if } n \equiv 1 \pmod 3 \\ -1 \text{ if } n \equiv -1 \pmod 3. \end{cases} \tag{A8}$$

Combining this information, we find

$$F(y;q) = \Delta(q^2) + 3\left(\sum_{n\equiv 1 (\mathrm{mod}\, 3)} \frac{y^n}{q^n - q^{-n}} - \sum_{n \equiv 2(\mathrm{mod}\, 3)} \frac{y^n}{q^n - q^{-n}}\right). \tag{A9}$$

As was said before, the right-hand side only converges for $|q| < |y| < |q|^{-1}$. To exploit the fact that F vanishes for $y = q$, which will yield the expression of $\Delta(q^2)$, we have to continue analytically by exhibiting the poles at $y = jq$ and j^2q. This is achieved by rewriting (A9) as

$$F(y;q) = \Delta(q^2) + 3\left(\sum_{\substack{n>0 \\ n\equiv 1(\mathrm{mod}\, 3)}} \frac{y^n q^n + y^{-n} q^{3n}}{q^{2n} - 1} - \sum_{\substack{n>0 \\ n \equiv 2(\mathrm{mod}\, 3)}} \frac{y^{-n} q^{3n} + y^n q^n}{q^{2n-1}} - \frac{yq}{y^2 + yq + q^2}\right). \tag{A10}$$

We can now set $y=q$. The left-hand side vanishes. Therefore, changing q^2 into q

$$\Delta(q)=1+6\left(\sum_{\substack{n>0\\ n\equiv 1(\mathrm{mod}\,3)}}\frac{q^n}{1-q^n}-\sum_{\substack{n>0\\ n\equiv 2(\mathrm{mod}\,3)}}\frac{q^n}{1-q^n}\right). \tag{A11}$$

Expanding the denominators and summing over n first yields the alternate expression

$$\Delta(q)=\sum_{m,n}q^{m^2+n^2+mn}=1+6\sum_{p=1}^{\infty}\frac{q^p}{1+q^p+q^{2p}}. \tag{A12}$$

We should have noted that, by rewriting m^2+n^2+mn as $\frac{1}{4}(2m+n)^2+\frac{3}{4}n^2$ and separating in the sum (A12) even and odd terms in n, $\Delta(q)$ can be expressed also as

$$\Delta(q)=\sum_{m,n}q^{\frac{1}{4}(2m-n)^2+\frac{3}{4}n^2}=\theta(1;q)\theta(1;q^3)+q\theta(q;q)\theta(q^3,q^3). \tag{A13}$$

This completes the proof of (3.18). We observe in passing that, since the distance of a vertex to the centre of one of the three adjacent upward pointing triangles is $1/\sqrt{3}$, one has the relation

$$\Delta(q)=\Delta(q^3)+2\Delta_1(q^3) \tag{A14}$$

which enables one to obtain for Δ_1 a relation similar to (A12)

$$\begin{aligned}\Delta_1(q)&=q^{1/3}[\theta(1;q)\theta(q^2;q^3)+\theta(q;q)\theta(q;q^3)]\\ &=3\left(\sum_{\substack{n>0\\ n\equiv 1(\mathrm{mod}\,3)}}(-1)^{n-1}\frac{q^{n/3}}{1-q^n}-\sum_{\substack{n>0\\ n\equiv 2(\mathrm{mod}\,3)}}(-1)^{n-1}\frac{q^{2n/3}}{1-q^n}\right).\end{aligned} \tag{A15}$$

We turn now to a similar expression for $\Delta(q)^2$. Although one could proceed by squaring the identity (A10), it is slightly easier to compute the logarithmic derivative of

$$f(y)=\theta(-yq^{-1/2};q^{1/2})=\prod_{n=1}^{\infty}(1-q^n)(1-y)\prod_{n=1}^{\infty}[(1-yq^n)(1-y^{-1}q^n)] \tag{A16}$$

i.e.

$$\begin{aligned}\varphi(y)&=\frac{y}{f(y)}\frac{\mathrm{d}f(y)}{\mathrm{d}y}=\sum_{n=1}^{\infty}\frac{q^n}{y-q^n}-\sum_{n=0}^{\infty}\frac{q^n}{y^{-1}-q^n}\\ &=\frac{1}{1-y^{-1}}+(y^{-1}-y)\sum_{n=1}^{\infty}\frac{q^n}{1-(y+y^{-1})q^n+q^{2n}}\end{aligned} \tag{A17}$$

$$\varphi(j)=\tfrac{1}{6}j(j-1)[2j+1+\Delta(q)]\qquad \varphi(j^2)=-\tfrac{1}{6}j^2(j^2-1)[2j+1-\Delta(q)].$$

Hence

$$\Delta^2(q)=3-6[\varphi^2(j)+\varphi^2(j^2)]. \tag{A18}$$

We now square (A17), and use the identities, valid for $m\neq n$,

$$\frac{1}{(y-q^n)(y-q^m)}=\frac{1}{(q^n-q^m)(y-q^n)}+\frac{1}{(q^m-q^n)(y-q^m)}$$

$$\frac{1}{(y-q^n)(y^{-1}-q^m)}=\frac{1}{1-q^{n+m}}\left(1+\frac{q^n}{y-q^n}+\frac{q^m}{y^{-1}-q^m}\right)$$

to write

$$\varphi(y)^2=\sum_{n=1}^{\infty}\left(\frac{q^{2n}}{(y-q^n)^2}+\frac{q^{2n}}{(y^{-1}-q^n)^2}-\frac{2nq^n}{1-q^n}\right)+\frac{1}{(1-y^{-1})^2}$$
$$+2\sum_{n=1}^{\infty}\frac{q^n}{(y-q^n)}\left(\sum_{\substack{m=1\\ m\neq n}}^{\infty}\frac{q^m}{q^n-q^m}-\sum_{m=0}^{\infty}\frac{q^{n+m}}{1-q^{n+m}}\right)$$
$$+2\sum_{n=0}^{\infty}\frac{q^n}{(y^{-1}-q^n)}\left(\sum_{\substack{m=0\\ m\neq n}}^{\infty}\frac{q^m}{q^n-q^m}-\sum_{m=1}^{\infty}\frac{q^{n+m}}{1-q^{n+m}}\right). \tag{A19}$$

The last two sums over m are respectively equal to $-(n-1)$ and $-n$. For $|q|<|y|<|q|^{-1}$, we then expand the denominators including y and resum in the opposite order, with the result that

$$\varphi(y)^2=\frac{1}{(1-y^{-1})^2}+\sum_{n=1}^{\infty}\left((n-1)\frac{q^n}{1-q^n}(y^n+y^{-n})-\frac{2nq^n}{1-q^n}-2\frac{q^ny^n+q^{2n}y^{-n}}{(1-q^n)^2}\right). \tag{A20}$$

Consequently, noting that $j^n+j^{-n}=3\delta_{n,0(\bmod 3)}-1$, from (A18)

$$\Delta^2(q)=1+12\left[\sum_{n=1}^{\infty}(1-3\delta_{n,0(\bmod 3)})\left(\frac{nq^n}{1-q^n}-\frac{2q^n}{(1-q^n)^2}\right)+\frac{2nq^n}{1-q^n}\right].$$

Taking finally into account that

$$\sum_{n=1}^{\infty}\frac{nq^n}{1-q^n}=\sum_{n=1}^{\infty}\frac{q^n}{(1-q^n)^2}$$

we cast this result in the form

$$\begin{aligned}\Delta^2(q)&=1+12\sum_{n=1}^{\infty}\left(\frac{nq^n}{1-q^n}-\frac{3nq^{3n}}{1-q^{3n}}\right)\\ &=1+12\sum_{n=1}^{\infty}\left(\frac{q^n}{(1-q^n)^2}-\frac{3q^{3n}}{(1-q^{3n})^2}\right)\end{aligned} \tag{A21}$$

which is the desired identity (3.19). It states that the coefficient of q^N in the expansion of $\Delta^2(q)$, for N positive, is 12 times the sum of its divisors which are not multiples of three. Obviously the method used here could have been applied to $\theta(1;q)^4$ by evaluating $\varphi^2(i)$. It would also seem possible to expres similarly higher powers of $\Delta(q)$ or $\theta^2(1;q)$. We finally remark that $\Delta_1(q)^2$ also has a simple expansion

$$\begin{aligned}\Delta_1(q)^2&=9\sum_{n\equiv 1(\bmod 3)}\frac{q^{2n/3}}{(1-q^n)^2}\\ &=9q^{2/3}\sum_{p=0}^{\infty}\left(\frac{q^{2p}}{(1-q^{3p+1})^2}+\frac{q^{4p+2}}{(1-q^{3p+2})^2}\right).\end{aligned} \tag{A22}$$

References

[1] Rayleigh Lord 1945 *The theory of sound* (New York: Dover)
[2] Berry M V 1981 *Ann. Phys., NY* **131** 163
[3] Kuttler J R and Sigillito V G 1984 *SIAM Rev.* **26** 163

[4] Pinsky M A 1980 *SIAM J. Math. Anal.* **11** 819
[5] Balian R and Bloch C 1970 *Ann. Phys., NY* **60** 401; 1971 *Ann. Phys., NY* **64** 271; 1972 *Ann. Phys., NY* **69** 76
[6] Weil A 1984 *Number Theory* (Basle: Birkhäuser)
[7] Coxeter H S M 1973 *Regular polytopes* (New York: Dover)
[8] Richens P J and Berry M V 1981 *Physica* **2D** 495
[9] Turner J W 1984 *J. Phys. A: Math. Gen.* **17** 2791
[10] Berard P 1979 *C.R. Acad. Sci., Paris* **288A** 1059
[11] Hardy G H and Wright E M 1979 *An introduction to the theory of numbers* (Oxford: Oxford University Press)
[12] Erdelyi A, Magnus N, Oberhettinger F and Tricomi F G 1955 *Higher transcendental functions* vol III (New York: McGraw-Hill)
[13] Andrews G E 1976 *The theory of partitions* (Reading, MA: Addison-Wesley)
[14] Slater L J 1966 *Generalized hypergeometric functions* (Cambridge: Cambridge University Press)
[15] Blanchard A 1969 *Initiation à la théorie analytique des nombres premiers* (Paris: Dunod)
[16] Serre J P 1970 *Cours d'arithmétique* (Paris: Presses Universitaires de France)