

# Discrete symmetries in the Weyl expansion for quantum billiards

Nicolas Pavloff

Division de Physique Théorique<sup>1</sup>, Institut de Physique Nucléaire, F-91406 Orsay Cedex, France

## abstract

We consider 2 and 3 dimensional quantum billiards with discrete symmetries. The boundary condition is either Dirichlet or Neumann. We derive the first terms of the Weyl expansion for the level density projected onto the irreducible representations of the symmetry group. The formulae require only the knowledge of the character table of the group and the geometrical properties (such as surface, perimeter etc ...) of sub-parts of the billiard invariant under a group transformation.

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<sup>1</sup>Unité de Recherche des Universités Paris XI et Paris VI associée au CNRS.

Billiards have been extensively studied in the context of quantum chaos, both from the semi-classical point of view (periodic orbit theory, see e.g. Ref. [1]) and using random matrix theory (for a review see [2]). In these two approaches it is important to subtract the smooth part of the level density in order to study the oscillations (trace formula) or the short range fluctuations (random matrices) around the average behaviour. The asymptotic behaviour of the smooth part of the level density — characterized by the Weyl expansion — is also of interest in a great variety of other physical and mathematical problems (see Refs. [3, 4, 5, 6, 7, 8]).

In this letter we study two and three dimensional billiards : a quantum particle is enclosed in a compact region  $B$  of space and we impose to its wave-function  $\psi$  Dirichlet or Neumann boundary conditions on the frontier  $\partial B$  ( $\partial B$  may or may not be a smooth manifold). Thus  $\psi$  verifies the following equation :

$$\begin{aligned} (\Delta + k^2)\psi &= 0 & \text{inside } B, \\ \psi &= 0 & \text{on } \partial B \quad (\text{Dirichlet}) \\ \mathbf{n} \cdot \nabla \psi &= 0 & \text{on } \partial B \quad (\text{Neumann}). \end{aligned} \quad (1)$$

We will assume that  $B$  remains invariant under a discrete point group  $\mathcal{G}$ . Then the eigenfunctions  $\{\psi_n\}_{n>0}$  and eigenvalues  $\{k_n\}_{n>0}$  can be classified according to the different irreducible representations (irreps) of the group. We label these irreps by an index ( $\alpha$ ), each has a dimension  $d^\alpha$ . Hence the total level density  $\rho(k)$  can be written as :

$$\rho(k) = \sum_{\alpha=1}^r \rho^\alpha(k), \quad (2)$$

where  $r$  is the total number of non-equivalent irreps of  $\mathcal{G}$ , and  $\rho^\alpha(k)$  is the density of levels belonging to irrep  $\alpha$  :

$$\rho^\alpha(k) = d^\alpha \sum_{n=0}^{\infty} \delta(k - k_n^\alpha). \quad (3)$$

$\rho(k)$  (resp.  $\rho^\alpha(k)$ ) can be separated in a smooth function of  $k$ ,  $\bar{\rho}(k)$  (resp.  $\bar{\rho}^\alpha(k)$ ) plus an oscillating part  $\tilde{\rho}(k)$  (resp.  $\tilde{\rho}^\alpha(k)$ ). The study of the oscillating part  $\tilde{\rho}^\alpha$  needs a careful treatment and has been addressed in Ref. [9, 10, 11, 12]. Our aim is to write the first terms of an explicit Weyl expansion for  $\bar{\rho}^\alpha(k)$  :

$$\bar{\rho}^\alpha(k) = \bar{\rho}_0^\alpha(k) + \bar{\rho}_1^\alpha(k) + \dots \quad (4)$$

In 3D  $\bar{\rho}_0^\alpha(k)$  is a volume term of order  $k^2$ ,  $\bar{\rho}_1^\alpha(k)$  is a surface term of order  $k$  and the next order is a constant (order zero in  $k$ ) edge term  $\bar{\rho}_2^\alpha$ . In the following we specialize the periodic orbit theory initiated in Ref. [9] to the simple case of zero length trajectories and treat the boundary conditions by using the Balian and Bloch method [5]. We will derive the formulae in the case of three dimensional billiards and only state the two dimensional results.

The projector onto an irreducible invariant subspace ( $\alpha$ ) is written as [13] :

$$P^\alpha = \frac{d^\alpha}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \chi^\alpha(g) U^\dagger(g), \quad (5)$$

where  $|\mathcal{G}|$  is the order of the group,  $\chi^\alpha(g)$  is the character of group element  $g$  in irrep  $(\alpha)$  and  $U(g)$  is the operator representing the action of  $g$  in Hilbert space. The projected level density is then (see [9]):

$$\rho^\alpha(k) = -\frac{2k}{\pi} \text{Im Tr}\{P^\alpha G(k + i0^+)\}, \quad (6)$$

where  $G(k + i0^+)$  is the retarded Green function of our problem; for simplicity we will drop the argument in the following. According to the ideas of Balian and Bloch,  $G$  is written as the free Green function  $G_0$  plus a correcting term:

$$G = G_0 + G_1. \quad (7)$$

We will here only need the explicit expression of  $G_1$  for short trajectories near the boundary  $\partial B$ . In this case it can be approximated using the method of images:

$$\langle r | G_1 | r' \rangle = \epsilon \langle r | G_0 | r'_1 \rangle, \quad (8)$$

where  $\epsilon = \pm 1$  for Dirichlet or Neumann boundary conditions and  $r'_1$  is the symmetric of point  $r'$  with respect to the plane tangent to  $\partial B$ . Note that (8) is properly defined only if  $r$  and  $r'$  are close to each other and close to the boundary. (8) is the leading correction (in the  $k$  expansion) to  $G_0$  arising near the boundary. A more systematic expansion can be found in Ref. [5]. In the Balian-Bloch terminology, we only consider the first term of the multiple scattering expansion and furthermore restrict ourselves to zero length orbits (or high wave vector).

In three dimensions,  $G_0$  contributes to the total level density with a volume term  $\bar{\rho}_0(k) = V k^2 / 4\pi^2$  ( $V$  being the volume of the billiard),  $G_1$  gives the surface term  $\bar{\rho}_1(k)$  and the next order  $\bar{\rho}_2$  is obtained by pursuing the multiple scattering expansion. We shall not consider higher orders in the expansion. Surprisingly enough, when computing the symmetry-projected terms ( $\bar{\rho}_0^\alpha$ ,  $\bar{\rho}_1^\alpha$  and  $\bar{\rho}_2^\alpha$ ), we need not know the form of the Green function to a better approximation than (7,8).

The contribution of  $G_0$  to the level density (6) is (using (5))

$$-\frac{2k}{\pi} \frac{d^\alpha}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \chi^\alpha(g) \text{Im} \int d^3r \langle gr | G_0 | r \rangle, \quad (9)$$

and the non-oscillating part of this expression is given by the quasi zero length trajectories going from  $r$  to  $gr$ . In 3D the elements of a point group  $\mathcal{G}$  can be either symmetries with respect to a plane, rotations or improper rotations (ie product of elements of the two first types); and orbits going from  $r$  to  $gr$  do not all contribute at the same order in the Weyl expansion:

(i) If  $g = e$  is the identity, then  $er = r$  for all points in  $B$  and (9) gives the projected volume term  $\bar{\rho}_0^\alpha(k)$ .

(ii) If  $g$  is a symmetry with respect to a plane, it leaves invariant a surface of area  $S_g$  (intersection of the plane of symmetry with  $B$ ) and then the corresponding term in (9) will contribute to  $\bar{\rho}_1^\alpha$ .

(5)

(iii) If  $g$  is a rotation, its invariant points in  $B$  are located on a segment of length  $L_g$  and we will have an edge contribution to  $\bar{\rho}_2^\alpha$ .

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Terms arising from improper rotations in (9) do not contribute at order  $\bar{\rho}_2^\alpha$  and we will not consider them here. From (9) we can readily write the symmetry projected volume term (the first term in the Weyl expansion) :

(6)

$$\bar{\rho}_0^\alpha(k) = \frac{(d^\alpha)^2}{|G|} \bar{\rho}_0(k). \quad (10)$$

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This formula is quite general and holds also for smooth potentials. A similar expression can be derived for continuous symmetry groups as well : the discrete sum in (5) is simply replaced by an integration on the invariant measure of the group. To fix the ideas, if we consider a system with 5 fold and 1 fold degenerate levels, formula (10) implies that roughly speaking, the 5 fold degenerate levels will contribute 25 times more to the level density than the singly degenerate levels (due to the coefficient  $(d^\alpha)^2$  in (10)). This contribution comprises a trivial factor 5 coming from the degeneracy of the levels. But the factor 5 remaining ( $25 = 5 \times 5$ ) is more surprising : when choosing a level at random in the spectrum, the probability is approximatively 5 times bigger for drawing a 5 fold degenerate level than for a singly degenerate level.

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The contribution of  $G_1$  to the level density (6) is of the same type as Eq. (9). There similarly, the identity, symmetries with respect to a plane and rotations do not contribute at the same order. The identity gives a surface contribution  $(d^\alpha)^2 \bar{\rho}_1 / |G|$  (as for the volume term (10) arising from  $g = e$  in (9)). Symmetries contribute to  $\bar{\rho}_2^\alpha$  and we will not consider the effects of rotations (contributing at higher order). The term following  $G_1$  as given by (8) in the multiple reflexion expansion contributes to the total level density at order  $\bar{\rho}_2$ . Its contribution will be weighted by a factor  $(d^\alpha)^2 / |G|$  when projected onto a given irrep (this again comes from  $g = e$  in (5) while other elements of the group contribute at higher orders).

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Gathering all the contributions we get for the surface and edge terms :

(9)

$$\bar{\rho}_1^\alpha(k) = \frac{(d^\alpha)^2}{|G|} \bar{\rho}_1(k) - \frac{2k d^\alpha}{\pi |G|} \sum_{g \in G_{sym.}} \chi^\alpha(g) \text{Im} \int d^3 r \langle g r | G_0 | r \rangle, \quad (11)$$

$$\begin{aligned} \bar{\rho}_2^\alpha(k) = \frac{(d^\alpha)^2}{|G|} \bar{\rho}_2(k) - \frac{2k d^\alpha}{\pi |G|} \sum_{g \in G_{rot.}} \chi^\alpha(g) \text{Im} \int d^3 r \langle g r | G_0 | r \rangle \\ - \frac{2k d^\alpha}{\pi |G|} \sum_{g \in G_{sym.}} \chi^\alpha(g) \text{Im} \int d^3 r \langle g r | G_1 | r \rangle. \end{aligned} \quad (12)$$

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In (11,12) the integration must be restricted to quasi-zero length trajectories.  $\sum_{g \in G_{rot.}}$  indicates a sum restricted to the rotations of the group (the same convention holds for  $\sum_{g \in G_{sym.}}$ ). To be specific we will compute one of the integrals in (11,12). Let us consider for instance the last term of the r.h.s. of Eq. (11). The integral  $\int d^3 r$  can be separated in a surface integral  $\int dx dy$  along the invariant symmetry plane plus a term  $\int dz$  along the normal to this plane. Then the modulus  $\|gr - r\| = 2|z|$  and the free Green function reads (see e.g. Ref. [14])

section  
e to  $\bar{\rho}_1^\alpha$ .

$$\langle g\mathbf{r}|G_0|\mathbf{r}\rangle = -\frac{e^{i\mathbf{k}|\mathbf{g}\mathbf{r}-\mathbf{r}|}}{4\pi|\mathbf{g}\mathbf{r}-\mathbf{r}|} = -\frac{e^{2i\mathbf{k}|z|}}{8\pi|z|}. \quad (13)$$

Hence the integral over  $dx dy$  will give a factor  $S_g$  (the area of the invariant surface) and the imaginary part of the integral over  $dz$  will give

$$-\frac{1}{8\pi} \int_{-\infty}^{+\infty} dz \frac{\sin(2k|z|)}{|z|} = -\frac{1}{8}. \quad (14)$$

Thus the total surface projected term (11) reads :

$$\bar{\rho}_1^\alpha(k) = \frac{(d^\alpha)^2}{|\mathcal{G}|} \bar{\rho}_1(k) + \frac{d^\alpha}{|\mathcal{G}|} \sum_{g \in \mathcal{G}_{sym.}} \chi^\alpha(g) \frac{k S_g}{4\pi}. \quad (15)$$

We note that : (i) if a class of  $\mathcal{G}$  contains one symmetry it is only formed by symmetries ; (ii)  $\chi^\alpha(g) S_g$  is a class function, i.e. it takes the same value for all symmetries belonging to the same class  $C$  (we note  $\chi^\alpha(C) S_C$  the value of the class function). Hence (15) can be written as a sum over those classes of the group which are formed by symmetries with respect to a plane (noted  $\sum_{C_{sym.}}$  below) :

$$\bar{\rho}_1^\alpha(k) = \frac{(d^\alpha)^2}{|\mathcal{G}|} \bar{\rho}_1(k) + \frac{d^\alpha}{|\mathcal{G}|} \sum_{C_{sym.}} \chi^\alpha(C) |\mathcal{G}_C| \frac{k S_C}{4\pi}. \quad (16)$$

In (16)  $|\mathcal{G}_C|$  is the number of elements of the group belonging to class  $C$ .

Similar computations yield for the edge terms :

$$\bar{\rho}_2^\alpha(k) = \frac{(d^\alpha)^2}{|\mathcal{G}|} \bar{\rho}_2(k) + \frac{d^\alpha}{|\mathcal{G}|} \sum_{C_{rot.}} \chi^\alpha(C) |\mathcal{G}_C| \frac{L_C}{4\pi \sin^2(\frac{\beta_C}{2})} + \epsilon \frac{d^\alpha}{|\mathcal{G}|} \sum_{C_{sym.}} \chi^\alpha(C) |\mathcal{G}_C| \frac{\partial S_C}{8\pi}. \quad (17)$$

In (17)  $\beta_C$  is the angle of rotation, common (modulo an irrelevant sign) to all the rotations belonging to a given class  $C$  and  $L_C$  is the common length of the invariant segments. Here also we use the fact that if a class contains one rotation, then it contains only rotations.  $\partial S_C$  is the common perimeter of the surfaces invariant under the symmetries belonging to the same class (i.e.  $\partial S_C$  is the perimeter of  $S_C$ ).

Formulae (10), (16) and (17) (together with their 2D counterparts (18) and (19)) are the most important results of this paper. They allow to compute the first terms of the symmetry projected Weyl expansion knowing only the character table of the group and the surfaces, lengths and perimeters of sub-parts of  $B$  invariant under a given class of group transformations. Note that using elementary group theoretical properties of the character table (see e.g. Ref. [13]) one recovers the total smooth level density when summing the different projected terms.

In two dimensions, the present formalism allows to determine the value of  $\bar{\rho}_0^\alpha(k)$  (which is now a surface term) and of  $\bar{\rho}_1^\alpha(k)$  (the perimeter correction). The formulae read :

$$\bar{\rho}_0^\alpha(k) = \frac{(d^\alpha)^2}{|\mathcal{G}|} \bar{\rho}_0(k), \quad (18)$$

$$\bar{\rho}_1^\alpha(k) = \frac{(d^\alpha)^2}{|\mathcal{G}|} \bar{\rho}_1(k) + \frac{d^\alpha}{|\mathcal{G}|} \sum_{C_{sym.}} \chi^\alpha(C) |\mathcal{G}_C| \frac{L_C}{2\pi}. \quad (19)$$

In (18,19)  $\bar{\rho}_0(k) = Sk/2\pi$  ( $S$  being the area of the billiard) is the total surface term and  $\bar{\rho}_1(k) = \epsilon L/4\pi$  ( $L$  is the perimeter) the total perimeter term.  $L_c$  is the common length of the segments invariant under the symmetries belonging to the class considered.

An alternative method for deriving the above results would be to work in reduce configuration space, to find out for each irrep which are the boundary conditions on the elementary cell and to work out the corresponding Weyl expansion (as was done in [15] for instance). But for some symmetry groups the boundary conditions on the elementary cell relevant for each irrep can be cumbersome (see below the example of the icosahedron) and also the corresponding Weyl expansion might not be known up to order  $\bar{\rho}_2^{\alpha}(k)$ : some irreps lead to mixed Neumann-Dirichlet conditions or impose phase-shifts when going from one boundary of the elementary cell to an other (this is the case for the rather simple group  $C_{3v}$ ). The method presented here has the advantage of giving simple and easily applied formulae that do not require detailed knowledge of the reduced boundary condition.

As an illustration let us consider a three dimensional icosahedral billiard with Dirichlet boundary conditions. This billiard was studied in [16] as a model for faceted metal clusters. The first 565 quantum levels were determined numerically (counting the degeneracies this leads to 2094 available states). The total symmetry group of the icosahedron is  $\mathcal{I}_h$ ; to simplify the presentation we will consider here only its subgroup  $\mathcal{I}$  formed by 60 rotations.  $\mathcal{I}$  has 5 classes and 5 non equivalent irreps, we will present only the results for one of the irreps which has dimension  $d^{\alpha} = 3$  (see table 1). In order to compare the numerical results with the predictions of Eq. (10), (16) and (17) we focus on the cumulated level density :

$$\bar{N}^{\alpha}(k) = \int_0^k \bar{\rho}^{\alpha}(k') dk' = \bar{N}_0^{\alpha}(k) + \bar{N}_1^{\alpha}(k) + \bar{N}_2^{\alpha}(k) + \bar{N}_3^{\alpha}(k) + \dots \quad (20)$$

From Ref. [6] we know the total —i.e. summed over all the irreps— terms  $\bar{N}_0$ ,  $\bar{N}_1$  and  $\bar{N}_2$  (the explicit expression is given in [16]).  $\mathcal{I}$  contains no symmetry and we can apply formulae (16,17) if knowing the length of the segments invariant under rotations (they are listed on table 1). The comparison of the numerical  $N^{\alpha}$  — which is a staircase function — with its smooth approximation  $\bar{N}_0^{\alpha} + \bar{N}_1^{\alpha} + \bar{N}_2^{\alpha}$  (from (10,16,17)) is shown Fig. 1. The difference is also plotted on this figure : as expected it is of order zero in  $k$ , and the amplitude of the oscillations is of order of the degeneracy  $d^{\alpha} = 3$ . A simple fit gives the value of the constant next order  $\bar{N}_3^{\alpha}(k) \simeq 0.288$ . The same agreement is also obtained for the other irreps of  $\mathcal{I}$  or when studying the irreps of the total group  $\mathcal{I}_h$ . It is interesting to note that the boundary conditions to be applied on the elementary cell when studying the different irreps of  $\mathcal{I}$  and  $\mathcal{I}_h$  are very difficult to determine. The method exposed here uses the character table of the group which comprises the necessary information in an easily accessible form.

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## Table captions

**Table 1.** Characters of the classes of  $\mathcal{I}$  for the irrep considered in the text. For the designation of the classes we use the conventions of Ref. [17].  $L_c$  is for each class (except for the identity) the length of the invariant segments.  $L_c$  is given in units of the edge length.

Classes	$1 C_1 = \{e\}$	$12 C_5$	$12 C_5^2$	$15 C_2$	$20 C_3$
$\chi^\alpha(C)$	3	$\frac{1-\sqrt{5}}{2}$	$\frac{1+\sqrt{5}}{2}$	-1	0
$L_c$	-	$\sqrt{\frac{5+\sqrt{5}}{2}}$	$\sqrt{\frac{5+\sqrt{5}}{2}}$	$\frac{1+\sqrt{5}}{2}$	$\frac{2}{\sqrt{3(3-\sqrt{5})}}$

## Figure captions

**Figure 1.** bottom part :  $N^\alpha(k)$  (staircase function) and its smooth approximation  $\bar{N}_0^\alpha + \bar{N}_1^\alpha + \bar{N}_2^\alpha$  as a function of  $k$ .  $k$  is given in units of the inverse length of the edge of the icosahedron. Top part : difference of the two quantities  $\Delta N^\alpha = N^\alpha - (\bar{N}_0^\alpha + \bar{N}_1^\alpha + \bar{N}_2^\alpha)$  as a function of  $N^\alpha$ . The thin horizontal line is the mean value of  $\Delta N^\alpha$  ( $\simeq 0.288$ ). The bottom plot is limited to the first 30 levels for legibility. The upper part concerns the first 100 levels (i.e. the first 300 quantum states).

