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Principal vectors of crystallographic groups and applications

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For a crystallographic group $\mathfrak{G}$ acting on an n-dimensional Euclidean space we consider the $\mathfrak{G}$-invariant linear elliptic differential operator P with constant coefficients and to it the $\mathfrak{G}$-automorphic eigenvalue problem $P[\psi] + \mu\psi = 0$. $N(\lambda)$ is the number of all eigenvalues μ smaller than or equal to the "frequency bound" λ^q (q: order of P). Earlier we found the asymptotic estimation $N(\lambda) \sim c_0 \cdot \lambda^n + c_1 \cdot \lambda^{n-1}$ (c_0, c_1: certain volumina). Furthermore, $N(\lambda)$ was interpreted as the number of so-called principal classes of principal lattice vectors within a convex domain. In this paper we demonstrate these results for the case $n = 2$ for two representative crystallographic groups $\mathfrak{G}$ and the assigned lattices. Above all we demonstrate a counting method for an exact estimation of $N(\lambda)$ if λ is not too big. In an analogous way we can treat all the 230 space groups of crystallography. It will be seen that these applications are brought about by the so-called principal vectors of these lattices.

0. Introduction

To follow this paper the consideration of Günther's [9] and my publication [3] is recommendable but is not a condition. The theory of these publications is repeated here partly but the actual aim is to demonstrate this theory by crystallographic groups.

Let $\mathfrak{G}$ be a properly discontinuous group of affine transformations acting on an n-dimensional affine space $\mathfrak{V}$. The invariant subgroub $\mathfrak{T} \subset \mathfrak{G}$ of all translation elements of $\mathfrak{G}$ defines a lattice $\Gamma \subset \mathfrak{V}$. To Γ is assigned the dual lattice Γ^* in the dual space $\mathfrak{V}^*$ to $\mathfrak{V}$. Günther introduced the notion "principal vector" of Γ^* and, by means of a certain equivalence relation between such vectors, also what he named "principal classes" in Γ^* (see [9]). Section 1 of this paper contains the definitions of such vectors and classes and their illustrations in a 2-dimensional Euclidean space $\mathfrak{V}^* = \mathbf{E}^2$ for the case of two representative crystallographic groups $\mathfrak{G}$.

Let P be a $\mathfrak{G}$-invariant self-adjoint linear elliptic differential operator with constant coefficients, $P[\psi] + \mu\psi = 0$ a $\mathfrak{G}$-automorphic eigenvalue problem (ψ: $\mathfrak{G}$-automorphic function on $\mathfrak{V}$). Let $N(\lambda)$ be the number of such eigenvalues μ which are equal to, or smaller than, the "frequency bound" λ^q (q: order of P). In [3,4] we found an interpretation of $N(\lambda)$ as a certain number of principal classes within a convex domain $\lambda \cdot \mathbf{D}$ in which $\mathbf{D} \subset \mathfrak{V}^*$ is an n-dimensional gauge domain defined by the principal part of P and $\lambda \cdot \mathbf{D}$ means the homothetical expansion of $\mathbf{D}$ with the factor λ. This interpretation opened two possibilities to seize $N(\lambda)$:

– In [3,4] $N(\lambda)$ is developed by the asymptotic expansion $N(\lambda) = c_0\lambda^n + c_1\lambda^{n-1} + O(\lambda^{n+2-2/(n+1)})$ where c_0 and c_1 are the volumina of $\mathbf{D}$ and of the $(n-1)$-dimensional cut domain between $\mathbf{D}$ and certain eigenspaces through $O \in \mathfrak{V}^*$.

– For a not too big λ we find an exact estimation of $N(\lambda)$ by counting the principal classes within $\lambda \cdot \mathbf{D}$.

In section 2 of this paper we study the important function $N(\lambda)$ for the above mentioned case that $\mathfrak{V}^* = \mathbf{E}^2$, $\mathfrak{G}$ a crystallographic group and P a differential operator of the order $q = 2$. In the case that $\mathfrak{V}^* = \mathbf{E}^3$ is the 3-dimensional Euclidean space and $\mathfrak{G}$ is one of the 230 space groups, the investigation of $N(\lambda)$ is carried out analogously, even if P is of order $q > 2$.

1. The principal vectors and principal classes of a crystallographic group

1.1. CRYSTALLOGRAPHIC GROUPS $\mathfrak{G}$, THEIR POINT GROUPS $\mathfrak{L}$ AND INVARIANT SUBGROUPS $\mathfrak{T}$

A crystallographic group $\mathfrak{G}$ acts on an n-dimensional Euclidean space $\mathbf{E}^n$ (especially we look at $n = 2$ or 3). We should write the elements $S \in \mathfrak{G}$ as Seitz-symbols $S = (\sigma, \mathfrak{s})$ so that the origins and images $\mathfrak{x}$ and $\mathfrak{x}' \in \mathbf{E}^n$ will transform according to $\mathfrak{x}' = S\mathfrak{x} = (\sigma, \mathfrak{s})\mathfrak{x} = \sigma\mathfrak{x} + \mathfrak{s}$. σ is called the fixed point part and $\mathfrak{s}$ the translation part of $(\sigma, \mathfrak{s})$. For $R = (\rho, \mathfrak{r})$, $S \in \mathfrak{G}$ the composition rule "o" in $\mathfrak{G}$ is $R \circ S = (\rho \circ \sigma, \rho\mathfrak{s} + \mathfrak{r}) \in \mathfrak{G}$. If $e = \mathrm{id}$ is the identical fixed point part and $O \in \mathbf{E}^n$ the zero vector, then $E = (e, O) \in \mathfrak{G}$ is the identity element in $\mathfrak{G}$ and $S^{-1} = (\sigma^{-1}, -\sigma^{-1}\mathfrak{s}) \in \mathfrak{G}$ the invers of S.

Let

$$\mathfrak{L} = \{\sigma | \exists \mathfrak{s} \in \mathbf{E}^n, (\sigma, \mathfrak{s}) \in \mathfrak{G}\}$$

be the point group of $\mathfrak{G}$ and

$$\mathfrak{T} = \{(e, \mathfrak{t}) \in \mathfrak{G}\}$$

the invariant subgroup of all translation elements of $\mathfrak{G}$. The factor group $\mathfrak{G}/\mathfrak{T}$ has a finite order r and because of the well-known isomorphy $\mathfrak{G}/\mathfrak{T} \cong \mathfrak{L}$ the order of $\mathfrak{L}$ is also r. In the coset decomposition of $\mathfrak{G}$ relative to $\mathfrak{T}$,

$$\mathfrak{G} = \kappa(\sigma_1) + \ldots + \kappa(\sigma_r), \kappa(\sigma_\nu) = S_\nu \circ \mathfrak{T},$$

$(S_\nu = (\sigma_\nu, \mathfrak{s}_\nu) \in \mathfrak{G}; \nu = 1, \ldots, r)$ the elements of one and the same coset $\kappa(\sigma_\nu)$ have the same fixed point part σ_ν while different cosets have different such parts: $(\sigma_\nu, \mathfrak{s}_\nu) \circ (e, \mathfrak{t}) = (\sigma_\nu \circ e, \sigma_\nu \mathfrak{t} + \mathfrak{s}_\nu) = (\sigma_\nu, \mathfrak{s}_\nu + \mathfrak{t}') \in \kappa(\sigma_\nu)$ is valid for all $(e, \mathfrak{t}) \in \mathfrak{T}$.

1.2. THE LATTICE Γ AND ITS DUAL Γ^*

$\mathfrak{T}$ has n generators $(e, \mathfrak{b}_1), \ldots, (e, \mathfrak{b}_n)$ with n linear independent translation parts $\mathfrak{b}_k$ used to form a base bas $\mathbf{E}^n$ and the $\mathfrak{L}$-invariant n-dimensional lattice in $\mathbf{E}^n$,

$$\Gamma := \mathrm{orb}_{\mathfrak{T}}(O) = \{\mathfrak{t} = t^k \mathfrak{b}_k \in \mathbf{E}^n | t^k \in \mathbf{Z}\},$$

where $\mathrm{orb}_{\mathfrak{T}}(O)$ means the orbit of $O \in \mathbf{E}^n$ under the action of group $\mathfrak{T}$; $\mathbf{Z}$ is the set of all integers.

$\mathfrak{a}$ is called "belonging to $\sigma \in \mathfrak{L}$" if $(\sigma, \mathfrak{a}) \in \mathfrak{G}$. Together with $\mathfrak{a}$ also all vectors $\mathfrak{a} + \Gamma$ and only these are belonging to σ. So modulo Γ exactly one vector $\mathfrak{a}$ is belonging to σ and it will be hitherto and in future denoted as $\mathfrak{a} = \mathfrak{s}$. If $(\sigma_1, \mathfrak{s}_1)$, $(\sigma_2, \mathfrak{s}_2)$, $(\sigma_1 \circ \sigma_2, \mathfrak{s}) \in \mathfrak{G}$ then sometimes it is useful to think of the Frobenius congruence

$$\sigma_1 \mathfrak{s}_2 + \mathfrak{s}_1 \equiv \mathfrak{s} \bmod \Gamma.$$

As usually in crystallography we take up also the dual situation with respect to that above. So let

$$\Gamma^* := \{\mathfrak{u} = u_h \mathfrak{b}^h | u_h \in \mathbf{Z}\}, \quad \langle \mathfrak{b}^h, \mathfrak{b}_k \rangle = \delta^h_k,$$

be the dual lattice to Γ in $\mathbf{E}^n$. δ^h_k is Kronecker's symbol and $\langle\ ,\ \rangle$ the scalar product in $\mathbf{E}^n$. Now instead of $\sigma \in \mathfrak{L}$ we have to use the adjoint mapping σ^{T} to σ:

$$\sigma^{\mathrm{T}}: \mathbf{E}^n \to \mathbf{E}^n \quad \text{with} \quad \sigma^{\mathrm{T}} \mathfrak{v} = \mathfrak{v} \circ \sigma, \quad \mathfrak{v} \in \mathbf{E}^n.$$

1.3. THE PRINCIPAL VECTORS OF Γ^*

For a fixed lattice vector $\mathfrak{u} \in \Gamma^*$ let

$$\mathfrak{N}(\mathfrak{u}) := \{\sigma \in \mathfrak{L} | \sigma^{\mathrm{T}} \mathfrak{u} = \mathfrak{u}\}$$

be the isotropy group. We consider the function

$$\varphi_{\mathfrak{u}}(\mathfrak{x}) := \exp\{2\pi i \langle \mathfrak{u}, \mathfrak{x} \rangle\}, \quad \mathfrak{x} \in \mathbf{E}^n. \tag{1}$$

$\varphi_{\mathfrak{u}}$ is a $\mathfrak{T}$-automorphic function on $\mathbf{E}^n$: $\varphi_{\mathfrak{u}}(\mathfrak{x} + \mathfrak{t}) = \varphi_{\mathfrak{u}}(\mathfrak{x}) \forall \mathfrak{t} \in \Gamma$. Therefore, and because for $(\sigma, \mathfrak{s}) \in \mathfrak{G}$ the translation part $\mathfrak{s}$ modulo Γ is well-established by σ, the character of $\mathfrak{N}(\mathfrak{u})$,

$$\chi(\mathfrak{u}, \sigma) := \varphi_{\mathfrak{u}}(\mathfrak{s}),$$

is correctly defined.

DEFINITION

If $\chi(\mathfrak{u}, \cdot)$ is the principal character of $\mathfrak{N}(\mathfrak{u})$, i.e.

$$\chi(\mathfrak{u}, \sigma) = 1 \quad \forall \sigma \in \mathfrak{R}(\mathfrak{u}),$$

then $\mathfrak{u} \in \Gamma^*$ is called the principal lattice vector or also the principal lattice point.

1.4. THE PRINCIPAL CLASSES OF Γ^*

$\mathfrak{u}', \mathfrak{u} \in \Gamma^*$ are called equivalent, $\mathfrak{u}' \sim \mathfrak{u}$, if there is a point transform $\sigma \in \mathfrak{L}$ so that $\mathfrak{u}' = \sigma^{\mathrm{T}}\mathfrak{u}$. Therefore Γ^* is decomposed in equivalence classes $\mathfrak{k}(\mathfrak{u}) = \{\mathfrak{u}' \in \Gamma^* | \mathfrak{u}' \sim \mathfrak{u}\}$ with the representative $\mathfrak{u}$. Now from [9] we take the fact that $\mathfrak{k}(\mathfrak{u})$ contains only principal vectors if $\mathfrak{u}$ is principal, or only non-principal vectors if $\mathfrak{u}$ is non-principal.

DEFINITION

$\mathfrak{k}(\mathfrak{u}) \subset \Gamma^*$ is called a principal class if $\mathfrak{u} \in \Gamma^*$ is principal; its denotation in this case is $\mathfrak{k} = \mathfrak{h}$.

REMARK 1

Because ord $\mathfrak{L} = r$ is finite also $\mathfrak{k}(\mathfrak{u})$ is finite,

$$\mathfrak{k}(\mathfrak{u}) = \{\mathfrak{u}_1, \ldots, \mathfrak{u}_l\}, \quad l \leqslant r;$$

of course, $\mathfrak{u}$ is one of the $\mathfrak{u}_1, \ldots, \mathfrak{u}_l$.

1.5. DEMONSTRATION OF THE PRINCIPAL LATTICE VECTORS AND PRINCIPAL CLASSES FOR THE CRYSTALLOGRAPHIC GROUPS Δ^2_{pg} AND Δ^2_{p31m} IN THE 2-DIMENSIONAL EUCLIDEAN SPACE $\mathbf{E}^2$.

(a) The group $\mathfrak{G} = \Delta^2_{pg}$

The 2-dimensional Euclidean space we relate to the orthonormal base $\{0; \mathfrak{e}_1, \mathfrak{e}_2\}$ at the origin $0 \in \mathbf{E}^2$. Then by means of the coset decomposition of $\mathfrak{G}$ relative to its invariant subgroup $\mathfrak{T}$, the group Δ^2_{pg} is defined according to

$$\Delta^2_{pg} = \mathfrak{T} + (\alpha, \mathfrak{a}) \circ \mathfrak{T},$$

where

$$\mathfrak{T} = \{(e, \mathfrak{t}) \in \Delta^2_{pg} | \mathfrak{t} = t^1\mathfrak{e}_1 + (2t^2)\mathfrak{e}_2 \ \forall t^i \in \mathbf{Z}\}$$

and relative to $\{0; \mathfrak{e}_1, \mathfrak{e}_2\}$ the fixed point parts e, α are represented by the (2,2) matrices

$$e \stackrel{\sim}{\rightarrow} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \alpha \stackrel{\sim}{\rightarrow} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \tag{2}$$

and

$$\mathfrak{a} \equiv \mathfrak{e}_2 (\mathrm{mod}\ \mathfrak{t}) .$$

α is the reflection of $\mathbf{E}^2$ with respect to the $\mathfrak{e}_2$-axis and so Δ^2_{pg} is generated by the gliding reflection $A = (\alpha, \mathfrak{a})$ and two linearly independent translations, e.g. $(e, \mathfrak{e}_1)$, $(e, \mathfrak{e}_2)$.

The point group to Δ^2_{pg} is clearly

$$\mathfrak{L} = \{e, \alpha\} \quad \text{with} \quad r = \mathrm{ord}\ \mathfrak{L} = 2 .$$

The lattice $\Gamma \subset \mathbf{E}^2$ is now explained by

$$\Gamma = \{\mathfrak{t} = t^1 \mathfrak{b}_1 + t^2 \mathfrak{b}_2 | t^i \in \mathbf{Z}\} ,$$

where

$$\mathfrak{b}_1 = \mathfrak{e}_1 , \quad \mathfrak{b}_2 = 2\mathfrak{e}_2 ,$$

and

$$\text{bas}\ \Gamma = \{0; \mathfrak{b}_1, \mathfrak{b}_2\}$$

forms the lattice base for Γ. With respect to bas Γ the space $\mathbf{E}^2$ has the metric fundamental tensor $(g_{ij}) := (\mathfrak{b}_i \cdot \mathfrak{b}_j)$ ("·": scalar product),

$$(g_{ij}) = \begin{pmatrix} 1 & 0 \\ 0 & 4 \end{pmatrix} . \tag{3a}$$

To this covariant form g_{ij} we obtain the contravariant form

$$(g^{hk}) = \begin{pmatrix} 1 & 0 \\ 0 & 1/4 \end{pmatrix} . \tag{3b}$$

If we characterize the base vectors $\mathfrak{b}^h$ of the reciprocal base

$$\text{bas}\ \Gamma^* = \{0; \mathfrak{b}^1, \mathfrak{b}^2\}$$

by upper indices $h = 1, 2$ we can define this base by means of the pull-up method

$$\mathfrak{b}^h = g^{hk}\mathfrak{b}_k = g^{h1}\mathfrak{b}_1 + g^{h2}\mathfrak{b}_2 = \begin{cases} 1 \cdot \mathfrak{b}_1 = \mathfrak{e}_1 & \text{if } h = 1 , \\ 1/4\ \mathfrak{b}_2 = 1/2\mathfrak{e}_2 & \text{if } h = 2 . \end{cases} \tag{4}$$

REMARK 2

Conversely, the pull-down method

$$\mathfrak{b}_i = g_{ij}\mathfrak{b}^j \quad (i = 1, 2)$$

leads from bas Γ^* to bas Γ.

As the reciprocal lattice we obtain

$$\Gamma^* = \{\mathfrak{u} = u_1 \mathfrak{b}^1 + u_2 \mathfrak{b}^2 | u_i \in \mathbf{Z}\} . \tag{5}$$

With respect to the sum convention we write in short

$$\mathfrak{t} = t^i \mathfrak{b}_i \in \Gamma \quad \text{and} \quad \mathfrak{u} = u_h \mathfrak{b}^h \in \Gamma^* .$$

The equivalence classes $\mathfrak{k}(\mathfrak{u}) \subset \Gamma^*$ appear in two types depending on the number of elements in $\mathfrak{k}(\mathfrak{u})$:

$$\mathfrak{k}_1 = \mathfrak{k}(\mathfrak{u}) = \{\mathfrak{u}\} \quad \text{if} \quad \mathfrak{u} = u_2 \mathfrak{b}^2 , \quad u_2 \in \mathbf{Z} , \quad l_1 = \text{ord}\, \mathfrak{k}_1 = 1 ,$$

$$\mathfrak{k}_2 = \mathfrak{k}(\mathfrak{u}) = \{\mathfrak{u}, \alpha^{\mathrm{T}} \mathfrak{u}\} \quad \text{if} \quad \mathfrak{k}_1 \not\ni \mathfrak{u} \in \Gamma^* , \quad l_2 = \text{ord}\, \mathfrak{k}_2 = 2 . \tag{6}$$

The isotropy groups $\mathfrak{N}(\mathfrak{u})$ – as subgroups of $\mathfrak{L} = \{e, \alpha\}$ – can appear at the most in two cases, in fact here we have both:

$$\mathfrak{N}_1 = \mathfrak{N}(\mathfrak{u}) = \{e, \alpha\} \quad \text{if} \quad \mathfrak{u} \in \mathfrak{k}_1 ,$$

$$\mathfrak{N}_2 = \mathfrak{N}(\mathfrak{u}) = \{e\} \quad \text{if} \quad \mathfrak{u} \in \mathfrak{k}_2 .$$

The vector $\mathfrak{u} \in \Gamma^*$ is a principal vector if $\chi(\mathfrak{u}, \sigma) = \mathrm{e}^{2\pi i \langle \mathfrak{u}, \mathfrak{s} \rangle} = 1 \; \forall \sigma \in \mathfrak{N}(\mathfrak{u})$, where $(\sigma, \mathfrak{s}) \in \Delta^2_{pg}$:

(i) If $\mathfrak{u} = u_2 \mathfrak{b}^2 \in \mathfrak{k}_1$, then $\mathfrak{N}(\mathfrak{u}) = \mathfrak{N}_1 = \{e, \alpha\}$, and for e, α we have

$$e: \quad \chi(\mathfrak{u}, e) = \mathrm{e}^{2\pi i \langle \mathfrak{u}, \mathfrak{t} \rangle} = \mathrm{e}^{2\pi i \langle u_2 \mathfrak{b}^2, t^1 \mathfrak{b}_1 + t^2 \mathfrak{b}_2 \rangle} = \mathrm{e}^{2\pi i u_2 t^2} \; {}^{1)}$$
$$= \cos(2 u_2 t^2 \cdot \pi) = 1 \quad \forall u_2, t^2 \in \mathbf{Z} ,$$

$$\alpha: \quad \chi(\mathfrak{u}, \alpha) = \mathrm{e}^{2\pi i \langle \mathfrak{u}, \mathfrak{a} \rangle} = \mathrm{e}^{2\pi i \langle u_2 \mathfrak{b}^2, 1/2\, \mathfrak{b}_2 \rangle}$$
$$= \cos(u_2 \cdot \pi) = \begin{cases} 1 & \text{if } u_2 \text{ even} \\ -1 & \text{if } u_2 \text{ odd} \end{cases} .$$

(ii) If $\mathfrak{u} = u_h \mathfrak{b}^h \in \mathfrak{k}_2$, then $\mathfrak{N}(\mathfrak{u}) = \mathfrak{N}_2 = \{e\}$, and for e we have

$$e: \quad \chi(\mathfrak{u}, e) = \mathrm{e}^{2\pi i \langle u_h \mathfrak{b}^h, t^j \mathfrak{b}_j \rangle} = \mathrm{e}^{2\pi i (u_h t^h)} = 1 \quad \forall u_h \in \mathbf{Z} , \quad u_2 \neq 0 .$$

From (ii) follows that all lattice vectors $\mathfrak{u} \in \mathfrak{k}_2$ are principal vectors. From (i) follows that all lattice vectors $\mathfrak{u} = u_2 \mathfrak{b}^2 \in \mathfrak{k}_1$ are principal if u_2 is even, and non-principal if u_2 is odd. In summary all lattice vectors $\mathfrak{u} \in \Gamma^*$ are principal except for $\mathfrak{u} = u_2 \mathfrak{b}^2$ with u_2 odd.

Therefore,

$$\mathfrak{h}_1 = \{\mathfrak{u}\} \quad \text{if} \quad \mathfrak{u} = u_2 \mathfrak{b}^2 \quad \text{with } u_2 \in \mathbf{Z} \text{ even} ,$$

$$\mathfrak{h}_2 = \{\mathfrak{u}, \alpha^{\mathrm{T}} \mathfrak{u}\} \quad \text{if} \quad \mathfrak{u} = u_i \mathfrak{b}^i \quad \text{with } u_i \in \mathbf{Z} , \quad u_1 \neq 0 , \tag{7}$$

appear as principal classes $\mathfrak{h} \subset \Gamma^*$ of $\mathfrak{G} = \Delta^2_{pg}$.

In fig. 1 we see the reciprocal lattice Γ^* to Δ^2_{pg}. The principal lattice points are marked by symbols $A_1, A_2, A_3, B_1, \ldots$. Lattice points without a symbol are not prin-

[1] To the left: $e = \mathrm{id} \in \mathfrak{L}$, to the right: $\mathrm{e} = \exp$.

cipal. All the principal lattice points which are marked by one and the same symbol form exactly one principal class $\mathfrak{h}$ of Γ^*. Later, if we define for $\mathfrak{h}$ the class norm $\|\mathfrak{h}\|$, we will see that classes of the same norm are characterized by the same kernel letter, for instance A.

(b) The group $\mathfrak{G} = \Delta^2_{p31m}$

We introduce Δ^2_{p31m} by means of its coset decomposition

$$\Delta^2_{p31m} = \mathfrak{T} + (\alpha, \mathfrak{a}) \circ \mathfrak{T} + (\beta, \mathfrak{b}) \circ \mathfrak{T} + (\gamma, \mathfrak{g}) \circ \mathfrak{T} + (\delta, \mathfrak{d}) \circ \mathfrak{T} + (\zeta, \mathfrak{z}) \circ \mathfrak{T}$$

relative to its invariant subgroup

$$\mathfrak{T} = \{(e, \mathfrak{t}) \in \Delta^2_{p31m} | \mathfrak{t} = t^1\mathfrak{b}_1 + t^2\mathfrak{b}_2; t^i \in \mathbf{Z}\}$$

of all translation elements $(e, \mathfrak{t})$. Here $\{0; \mathfrak{b}_1, \mathfrak{b}_2\}$ shall be a hexagonal base in the 2-dimensional Euclidean space $\mathbf{E}^2$. Relative to $\{0; \mathfrak{b}_1, \mathfrak{b}_2\}$ the group elements $(\alpha, \mathfrak{a})$, $(\beta, \mathfrak{b}), \ldots, (\zeta, \mathfrak{z}) \in \Delta^2_{p31m}$ are given as the integral representation

$$e \simeq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \alpha \simeq \begin{pmatrix} 1 & 0 \\ -1 & -1 \end{pmatrix}, \quad \beta \simeq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma \simeq \begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix},$$

$$\delta \simeq \begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix}, \quad \zeta \simeq \begin{pmatrix} -1 & -1 \\ 0 & 1 \end{pmatrix};$$

$$\mathfrak{a}, \mathfrak{b}, \mathfrak{g}, \mathfrak{d}, \mathfrak{z} \equiv 0 \bmod \mathfrak{t}.$$

The group table of the point group

$$\mathfrak{L} = \{e, \alpha, \beta, \gamma, \delta, \zeta\}, \quad r = 6,$$

to Δ^2_{p31m} is shown in table 3.

From $\mathfrak{T}$ we obtain the hexagonal lattice

$$\Gamma = \{\mathfrak{t} = t^1\mathfrak{b}_1 + t^2\mathfrak{b}_2 | t^i \in \mathbf{Z}\}, \text{bas } \Gamma = \{0; \mathfrak{b}_1, \mathfrak{b}_2\},$$

and the reciprocal lattice

$$\Gamma^* = \{\mathfrak{u} = u_1\mathfrak{b}^1 + u_2\mathfrak{b}^2 | u^h \in \mathbf{Z}\}, \text{bas } \Gamma^* = \{0; \mathfrak{b}^1, \mathfrak{b}^2\},$$

where $\mathfrak{b}^1 = 4/3 \cdot \mathfrak{b}_1 + 2/3 \cdot \mathfrak{b}_2, \mathfrak{b}^2 = 2/3 \cdot \mathfrak{b}_1 + 4/3 \cdot \mathfrak{b}_2$.

The metric fundamental tensors $g_{ij} = \mathfrak{b}_i \cdot \mathfrak{b}_j$ or $g^{hk} = \mathfrak{b}^h \cdot \mathfrak{b}^k$ in $\mathbf{E}^2$ are

$$(g_{ij}) = \tfrac{1}{2}\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \quad \text{bas } \Gamma$$

with respect to

$$(g^{hk}) = \tfrac{2}{3}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \quad \text{bas } \Gamma^*$$

(relative to the orthonormal system $\{0; \mathfrak{e}_1, \mathfrak{e}_2\}$ we have $\mathfrak{b}_1 = \mathfrak{e}_1$, $\mathfrak{b}_2 = -\frac{1}{2} \cdot \mathfrak{e}_1 + \sqrt{3}/2 \cdot \mathfrak{e}_2$; $\mathfrak{b}^1 = \mathfrak{e}_1 + 1/\sqrt{3} \cdot \mathfrak{e}_2$, $\mathfrak{b}^2 = 2/\sqrt{3} \cdot \mathfrak{e}_2$).

Because of $\mathfrak{a}, \mathfrak{b}, \mathfrak{g}, \mathfrak{d}, \mathfrak{z} \equiv 0 \pmod{\mathfrak{t}}$ the equation $\chi(\mathfrak{u}, \sigma) = 1$ is valid $\forall \sigma \in \mathfrak{L}$, i.e. all the lattice vectors $\mathfrak{u} \in \Gamma^*$ and so all the equivalence classes $\mathfrak{k}(\mathfrak{u}) \subset \Gamma^*$ are principal.

The equivalence classes appear in three types, namely being of the orders $l = 1, 3, 6$:

$$\mathfrak{k}_1 = \{0\}; \quad \mathfrak{k}_3^{\pm} = \{\pm u(-2\mathfrak{b}^1 + \mathfrak{b}^2), \pm u(\mathfrak{b}^1 + \mathfrak{b}^2), \pm u(\mathfrak{b}^1 - 2\mathfrak{b}^2)\}, \quad 0 < u \in \mathbf{Z};$$

$$\begin{aligned} \mathfrak{k}_6 = \{&u_1\mathfrak{b}^1 + u_2\mathfrak{b}^2, u_1\mathfrak{b}^1 - (u_1 + u_2)\mathfrak{b}^2, u_2\mathfrak{b}^1 + u_1\mathfrak{b}^2, u_2\mathfrak{b}^1 - (u_1 + u_2)\mathfrak{b}^2 \\ &- (u_1 + u_2)\mathfrak{b}^1 + u_1\mathfrak{b}^2, -(u_1 + u_2)\mathfrak{b}^1 + u_2\mathfrak{b}^2\}, \quad u_i\mathfrak{b}^i \notin \mathfrak{k}_1, \mathfrak{k}_3^{\pm}. \end{aligned} \tag{8}$$

In fig. 3 we see the reciprocal lattice Γ^* to Δ^2_{p31m}. Principal lattice points are marked by symbols A; B_1, B_2; C; D_1, D_2; F; .... One and the same symbol marks all points of one and the same principal class. The same kernel letter, for instance B, characterizes classes of the same class norm which will be introduced in section 2.1(b).

2. $\mathfrak{G}$-automorphic eigenvalue problems and numbers of eigenvalues for crystallographic groups

Before we continue to investigate the examples $\mathfrak{G} = \Delta^2_{pg}$, Δ^2_{p31m} we should know something about the $\mathfrak{G}$-invariant differential operators and their numbers of eigenvalues from [3] or [4]:

2.1. $\mathfrak{G}$-AUTOMORPHIC EIGENVALUE PROBLEMS AND THE BELONGING NUMBERS OF EIGENVALUES

Let $\mathfrak{G}$ be a crystallographic group and P a $\mathfrak{G}$-invariant linear elliptic differential operator with constant coefficients. The order of P may be arbitrary (see [4]). But for simplification and shortness we restrict ourselves to operators of second order,

$$P = P^{hk} \frac{\partial^2}{\partial v^h \partial v^k} - 4\pi i P^h \frac{\partial}{\partial v^h} - 4\pi^2 P^0, \tag{9}$$

where relative to bas $\Gamma = \{0; \mathfrak{b}_1, \ldots, \mathfrak{b}_n\}$ the coefficients $P^{hk} = P^{kh}$, P^h are the contravariant coordinates of a given 2-, 1-fold tensor, respectively, and $P^0 = P^h P_h$. Here relative to bas $\Gamma^* = \{0; \mathfrak{b}^1, \ldots, \mathfrak{b}^n\}$ the P_h is defined by $P_h = P_{h\nu} P^\nu$ and $P_{h\nu}$ by

$P_{h\nu}P^{k\nu} = \delta_h^k$. Furthermore $\mathfrak{v} = v_h \mathfrak{b}^h$ is a covariantly written vector in $\mathbf{E}^n$. As the characteristic polynom to P we have

$$\begin{aligned} P(\mathfrak{v}) &= -P^{hk}v_h v_k + 4\pi P^h v_h - 4\pi^2 P^0 \\ &= -P^{hk}(v_h - 2\pi P_h)(v_k - 2\pi P_k) . \end{aligned} \tag{10}$$

REMARK 3

(a) $\{P^{hk}\}$ could be interpreted as the metric fundamental tensor $\{g^{hk}\}$ of the Euclidean space $\mathbf{E}^n$; then $\mathfrak{b}^h \cdot \mathfrak{b}^k = g^{hk} := P^{hk}$ is the scalar product of $\mathbf{E}^n$. (b) $\overline{P[\varphi]\psi - P[\psi]\bar{\varphi}}$ (φ, ψ: functions) can be written as a divergence term and so P is a formally self-adjoint operator. (c) P is $\mathfrak{G}$-invariant; that means $P[\psi \circ S] = P[\psi] \circ S \; \forall S \in \mathfrak{G}$.

Now we consider the $\mathfrak{G}$-automorphic eigenvalue problem

$$P[\psi] + \mu\psi = 0 , \quad \psi \in L_2(\mathfrak{G}) , \tag{11}$$

where $L_2(\mathfrak{G})$ is the Hilbert space over $\mathbf{C}$ of locally quadratically integrable $\mathfrak{G}$-automorphic functions. $\mathfrak{G}$-automorphic means $\psi(S\mathfrak{x}) = \psi(\mathfrak{x}) \forall S \in \mathfrak{G}$ and $\mathfrak{x} = x^h \mathfrak{b}_h \in \mathbf{E}^n$. Let $\operatorname{spec}_{\mathfrak{G}}(P)$ be the $\mathfrak{G}$-automorphic eigenvalue spectrum of (11). For an arbitrary but fixed given "frequency bound" λ^2 we consider the number

$$N(\lambda) = \operatorname{card}\{\mu \in \operatorname{spec}_{\mathfrak{G}}(P) | \mu \leqslant \lambda^2\}$$

of all eigenvalues μ of (11) below λ^2.

(a) The eigenvalues and eigenfunctions of (11)

Let $\mathfrak{h} = \{\mathfrak{u}_1, \ldots, \mathfrak{u}_l\} \subset \Gamma^*$ be a principal class, $\mathfrak{N}(\mathfrak{u}_1)$ the isotropy group of $\mathfrak{u}_1$. $(\mathfrak{L}/\mathfrak{N}(\mathfrak{u}_1))_{\mathrm{L}}$ the left coset decomposition of the point group $\mathfrak{L}$ of $\mathfrak{G}$ with respect to $\mathfrak{N}(\mathfrak{u}_1)$. Further let $\operatorname{rep}(\mathfrak{L}/\mathfrak{N}(\mathfrak{u}_1))_{\mathrm{L}} = \{\sigma_1, \ldots, \sigma_l\}$ be a system of representatives of this decomposition. The $\mathfrak{s}_1, \ldots, \mathfrak{s}_l$ are vectors belonging to $\sigma_1, \ldots, \sigma_l$, i.e. $S_\nu = (\sigma_\nu, \mathfrak{s}_\nu) \in \mathfrak{G}$; $\nu = 1, \ldots, l$. So we can introduce the "$\mathfrak{h}$-corresponding" functions

$$\psi_{\mathfrak{h}}(\mathfrak{x}) = \frac{1}{\sqrt{l}} \sum_{\nu=1}^{l} \varphi_{\mathfrak{u}_1}(S_\nu \mathfrak{x}) , \quad \mathfrak{x} = x^h \mathfrak{b}_h \in \mathbf{E}^n , \tag{12}$$

where $\varphi_{\mathfrak{u}}$ comes from (1).

We know that $\psi_{\mathfrak{h}}$ is a $\mathfrak{G}$-automorphic function and $P[\psi_{\mathfrak{h}}] = P(2\pi\mathfrak{u})\psi_{\mathfrak{h}}$ if $\mathfrak{u} \in \mathfrak{h}$ (see [3,9]). Therefore $\psi_{\mathfrak{h}}$ is the automorphic eigenfunction to the eigenvalue $\mu_{\mathfrak{h}} = -P(2\pi\mathfrak{u})$. Because of $P(\sigma^{\mathrm{T}}\mathfrak{v}) = P(\mathfrak{v}) \forall \sigma \in \mathfrak{L}$, $\mathfrak{v} = v_h \mathfrak{b}^h \in \mathbf{E}^n$, the characteristic polynom P is a class function $P(2\pi\mathfrak{h}) := P(2\pi\mathfrak{u})$ where $\mathfrak{u} \in \mathfrak{h}$. So we have $\mu_{\mathfrak{h}} = -P(2\pi\mathfrak{h})$ and according to [3] only these $\mu_{\mathfrak{h}}$ are eigenvalues of (9). Therefore

$$\operatorname{spec}_{\mathfrak{G}}(P) = \{\mu_{\mathfrak{h}} = -P(2\pi\mathfrak{h}) | \mathfrak{h} \in \mathfrak{H}\} \tag{13}$$

is valid; $\mathfrak{H}$ is the set of all principal classes of Γ^*.

(b) P-norm for vectors and classes

DEFINITION

$\|\mathfrak{v}\|^2 = -\frac{1}{(2\pi)^2} P(2\pi(\mathfrak{v}+\mathfrak{p})) = P^{hk} v_h v_k$ is called the P-norm of $\mathfrak{v} = v_h \mathfrak{b}^h \in \mathbf{E}^n$, $\mathfrak{p} = P_h \mathfrak{b}^h$.

$\|\mathfrak{v}\|$ is an $\mathfrak{L}$-automorphic function (see (19), (10)), i.e.

$$\|\sigma^{\mathrm{T}}\mathfrak{v}\| = \|\mathfrak{v}\| \quad \forall \sigma \in \mathfrak{L}.$$

Therefore $\|\mathfrak{u}_1\| = \ldots = \|\mathfrak{u}_l\| = \|\mathfrak{u}\|$ is valid for $\mathfrak{k}(\mathfrak{u}) = \{\mathfrak{u}_1, \ldots, \mathfrak{u}_l\}$ which justifies:

DEFINITION

$\|\mathfrak{k}(\mathfrak{u})\| = \|\mathfrak{u}\|$ is said to be the class norm of $\mathfrak{k}(\mathfrak{u})$.

This norm has the property: If $\|\mathfrak{k}(\mathfrak{u})\| \neq \|\mathfrak{k}(\mathfrak{u}')\|$ so $\mathfrak{k}(\mathfrak{u}) \neq \mathfrak{k}(\mathfrak{u}')$ but not vice versa: for $\mathfrak{k}(\mathfrak{u}) \neq \mathfrak{k}(\mathfrak{u}')$ could well be $\|\mathfrak{k}(\mathfrak{u})\| = \|\mathfrak{k}(\mathfrak{u}')\|$. In fig. 1 all principal classes of $\mathfrak{G} = \Delta^2_{pg}$ with the same class norm are marked with one and the same capital letter. Different indices characterize different classes. All principal lattice points of one and the same class are denoted by the same symbol. For instance the classes $\mathfrak{h}_2 = \{\mathfrak{b}^1, -\mathfrak{b}^1\}$, $\mathfrak{h}_1 = \{2\mathfrak{b}^2\}$ and $\mathfrak{h}'_1 = \{-2\mathfrak{b}^2\}$ have the common capital letter A, the principal points $\mathfrak{b}^1, -\mathfrak{b}^1; 2\mathfrak{b}^2; -2\mathfrak{b}^2$ have then the symbols $A_1, A_1; A_2; A_3$. The denotation in fig. 3 must be interpreted analogously.

By means of the class norm the eigenvalues $\mu_{\mathfrak{h}}$ from (13) can be written as

$$\mu_{\mathfrak{h}} = (2\pi)^2 \|\mathfrak{h} - \mathfrak{p}\|^2, \quad \mathfrak{p} = P_h \mathfrak{b}^h, \tag{14}$$

where $\mathfrak{h} - \mathfrak{p}$ is the class of all vectors $\mathfrak{u}_\nu - \mathfrak{p}$ $\forall \mathfrak{u}_\nu \in \mathfrak{h}$.

(c) $N(\lambda)$ as the number of principal classes $\mathfrak{h}$ contained in a certain convex domain $\lambda \cdot \mathbf{D} \subset \mathbf{E}^n$

DEFINITION

For $\lambda > 0$ we introduce in $\mathbf{E}^n$ the domains

$$\mathbf{D} = \left\{ \mathfrak{v} \in \mathbf{E}^n \middle| \|\mathfrak{v}\| \leqslant \frac{1}{2\pi} \right\}, \tag{15a}$$

$$\lambda \cdot \mathbf{D} = \left\{ \mathfrak{v} \in \mathbf{E}^n \middle| \|\mathfrak{v}\| \leqslant \frac{\lambda}{2\pi} \right\}, \tag{15b}$$

$$\mathfrak{p} + \lambda \cdot \mathbf{D} = \left\{ \mathfrak{v} \in \mathbf{E}^n \middle| \|\mathfrak{v} - \mathfrak{p}\| \leqslant \frac{\lambda}{2\pi} \right\} \tag{15c}$$

and call them the gauge domain, homothetical expansion of $\mathbf{D}$ with λ as a factor, and parallel translated domain along the vector $\mathfrak{p}$, respectively. According to [3], proposition 1, formula (25),

$$N(\lambda) = \text{card}\{\mathfrak{h} \in \mathfrak{H} | \mathfrak{h} \subset (\mathfrak{p} + \lambda \cdot \mathbf{D})\} \tag{16}$$

is valid.

REMARK 4

Here we have the essential fact that either $\mathfrak{h} \subset (\mathfrak{p} + \lambda \cdot \mathbf{D})$ or $\mathfrak{h} \cap (\mathfrak{p} + \lambda \cdot \mathbf{D}) = \emptyset$, with $\lambda \cdot \mathbf{D}$ being an $\mathfrak{L}$-invariant domain for all $\lambda > 0$.

By means of formula (16) we can ascertain $N(\lambda)$ exactly, so far as λ is not too big: we simply have to count all the principal classes $\mathfrak{h}$ within the domain $\mathfrak{p} + \lambda \cdot \mathbf{D}$ and of its boundary.

(d) The asymptotic estimation of $N(\lambda)$

$N(\lambda)$ can be written as a finite sum of Weyl sums, and by means of Landau's estimation of the lattice remainder we get

$$N(\lambda) = \frac{1}{r}\text{vol}_n(\mathbf{D}) \cdot \lambda^n + \frac{1}{r} \sum_{\sigma \in \mathfrak{L}_{n-1}} \text{vol}_{n-1}(\mathbf{D} \cap \mathfrak{V}^*(\sigma)) \cdot \delta_\sigma \cdot \lambda^{n-1} + O(\lambda^{n-2+2/(n+1)}) \,. \tag{17}$$

Symbols in (17)

(i) $\delta_\sigma = 0$ or 1 is Landau's δ-symbol; according to proposition 4 in [3] the relation $\delta_\sigma = 1$ is valid for $(\sigma, \mathfrak{s}) \in \mathfrak{G}$ if and only if there is a lattice vector $\mathfrak{t}_0 \in \Gamma$ with the property that $(\sigma, \mathfrak{s} + \mathfrak{t}_0)$ has a fixed point $\mathfrak{x}_0 \in \mathbf{E}^n$, i.e. $\sigma\mathfrak{x}_0 + \mathfrak{s} + \mathfrak{t}_0 = \mathfrak{x}_0$. (ii) $r = \text{ord}\ \mathfrak{L}$ is the number of elements of $\mathfrak{L}$. (iii) $\mathfrak{V}^*(\sigma) := \ker(\sigma^{\mathrm{T}} - \text{id})$ is the eigenspace of the eigenvalue 1 of σ^{T} if $\sigma \in \mathfrak{L}_{n-1} := \{\sigma \in \mathfrak{L} | \dim \mathfrak{V}^*(\sigma) = n-1\}$. (iv) $\text{vol}_n(\mathbf{D})$, $\text{vol}_{n-1}(\mathbf{D} \cap \mathfrak{V}^*(\sigma))$ are the n-, $(n-1)$-dimensional volumes of the gauge domain and of the cut domain $\mathbf{D} \cap \mathfrak{V}^*(\sigma) \subset \mathbf{E}^n$, respectively; according to the procedure in [9], [3] or [4] we have to regard here also that the volume definition in $\mathbf{E}^n$ is founded on the normalisation

$$\text{vol}_n(\mathfrak{F}(\Gamma^*)) = 1\,, \quad \text{vol}_{n-1}(\mathfrak{F}(\Gamma^* \cap \mathfrak{V}^*(\sigma))) = 1\,, \tag{18}$$

where $\mathfrak{F}(\Gamma^*)$, $\mathfrak{F}(\Gamma^* \cap \mathfrak{V}^*(\sigma))$ are the fundamental domains of the lattices Γ^*, $\Gamma^* \cap \mathfrak{V}^*(\sigma)$, respectively.

2.2. EIGENVALUE BEHAVIOUR IN (11) WITH RESPECT TO THE GROUPS Δ^2_{pg} AND Δ^2_{p31m}

(a) The group $\mathfrak{G} = \Delta^2_{pg}$

First we recall again (section 1.5(a)) the definitions of $\Delta^2_{pg} = \mathfrak{T} + (\alpha, \mathfrak{a}) \circ \mathfrak{T}$ and the terms $\mathfrak{L}$; Γ, Γ^*; (g_{ij}), (g^{hk}); $\mathfrak{N}_1$, $\mathfrak{N}_2$ and above all of $\mathfrak{h}_1$, $\mathfrak{h}_2$ from (7).

Eigenvalues and eigenfunctions of the Δ^2_{pg}-automorphic eigenvalue problem (11)

First we consider all Δ^2_{pg}-invariant differential operators P. The invariance condition $P[\psi \circ S] = P[\psi] \circ S \; \forall S = (\sigma, \mathfrak{s})$ (see remark 3(c)) means for the coefficients P^{hk} and P^h of P that

$$P^{hk}\sigma^i_h\sigma^j_k = P^{ij}, \quad P^h\sigma^i_h = P^i, \tag{19}$$

are valid for all $\sigma = (\sigma^i_h) \in \mathfrak{L} = \{e, \alpha\}$ – interpreted with respect to the base bas $\Gamma = \{0; \mathfrak{b}_1, \mathfrak{b}_2\} = \{0; \mathfrak{e}_1, 2\mathfrak{e}_2\}$. For $\sigma = \mathrm{e} = (\delta^i_h)$ (Kronecker's symbol) eqs. (19) are identities. For $\sigma = \alpha = (\alpha^i_h)$ (see (2)) we obtain from (19) the set of all Δ^2_{pg}-invariant operators in the general form,

$$P = P^{11}\partial_1^2 + P^{22}\partial_2^2 + 4\pi \mathrm{i} P^2\partial_2 - (2\pi P^2)^2/P^{22},$$

$$P^{11}, P^{22} > 0, P^2 \text{ arbitrary}, \quad \partial_h = \frac{\partial}{\partial v^h} \quad \text{and} \quad \mathfrak{v} = v^h\mathfrak{b}_h. \tag{20}$$

The assigned characteristic polynom then is

$$P(\mathfrak{v}) = -P^{11}v_1^2 - P^{22}v_2^2 + 4\pi P^2 v_2 - (2\pi P^2)^2/P^{22}, \quad \mathfrak{v} = v_h\mathfrak{b}^h, \tag{21}$$

and the P-norm of $\mathfrak{v}$ is

$$\|\mathfrak{v}\| = (P^{11}v_1^2 + P^{22}v_2^2)^{1/2} \quad \text{relative to } \{0; \mathfrak{b}^1, \mathfrak{b}^2\}. \tag{22}$$

For P from (20) we solve now the Δ^2_{pg}-automorphic eigenvalue problem $P[\psi] + \mu\psi = 0$ according to the formulas (12), (13) and (21). To write the formula (12) for $\mathfrak{h} = \mathfrak{h}_1, \mathfrak{h}_2$ from (7) we must be aware of the fact that

$$\mathrm{rep}(\mathfrak{L}/\mathfrak{R}(\mathfrak{u}))_{\mathrm{L}} = \begin{cases} \{e\} & \text{if} \quad \mathfrak{u} \in \mathfrak{h}_1, \\ \{e, \alpha\} & \phantom{\text{if}} \quad \mathfrak{u} \in \mathfrak{h}_2. \end{cases}$$

For $\psi_{\mathfrak{h}_i}(\mathfrak{x})$ and $\mu_{\mathfrak{h}_i}$ $(i = 1, 2)$,

$$\psi_{\mathfrak{h}_1}(\mathfrak{x}) = \varphi_{\mathfrak{u}}(E\mathfrak{x}) = \varphi_{\mathfrak{u}}(\mathfrak{x}), \quad E = (e, 0),$$

$$\mu_{\mathfrak{h}_1} = -P(2\pi\mathfrak{h}_1) = (2\pi)^2(P^{22}u_2^2 - 2P^2u_2 + (P^2)^2/P^{22}), \tag{23}$$

where

$$\mathfrak{u} = u_2\mathfrak{b}^2 \in \mathfrak{h}_1, u_2 \text{ even};$$

$$\psi_{\mathfrak{h}_2}(\mathfrak{x}) = \frac{1}{\sqrt{2}}(\varphi_{\mathfrak{u}}(E\mathfrak{x}) + \varphi_{\mathfrak{u}}(A\mathfrak{x})), \quad A = (\alpha, \mathfrak{a}),$$
$$= \frac{1}{\sqrt{2}}(\varphi_{\mathfrak{u}}(\mathfrak{x}) + \varphi_{\mathfrak{u}}(\alpha\mathfrak{x} + \mathfrak{a})),$$

$$\mu_{\mathfrak{h}_2} = -P(2\pi\mathfrak{h}_2) = (2\pi)^2(P^{11}u_1^2 + P^{22}u_2^2 - 2P^2u_2 + (P^2)^2/P^{22}), \tag{24}$$

where

$$\mathfrak{u} = u_i \mathfrak{b}^i \in \mathfrak{h}_2 .$$

If $\mathfrak{h}_1, \mathfrak{h}_2$ run through the set $\mathfrak{H}$ of all principal classes of Δ^2_{pg} we obtain all eigenvalues $\mu_{\mathfrak{h}}$ and eigenfunctions $\psi_{\mathfrak{h}}(\mathfrak{x})$ of the Δ^2_{pg}-automorphic eigenvalue problem (11).

The number $N(\lambda)$ of eigenvalues

We obtain the asymptotic estimation of $N(\lambda)$ from (17). There we have for $\mathfrak{G} = \Delta^2_{pg}$ the data $n = 2, r = 2; \delta_e = 1, \delta_\alpha = 0$. The latter is valid because (according to section 2.1(d)) $(e, 0)$ has a fixed point (choose $\mathfrak{t}_0 = 0$) but for $(\alpha, \mathfrak{a})$ there is no $\mathfrak{t}_0 \in \Gamma$ so that $(\alpha, \mathfrak{a} + \mathfrak{t}_0)$ has a fixed point. Furthermore we have

$$\mathbf{D} = \left\{ \mathfrak{v} \in \mathbf{E}^2 | P^{11} v_1^2 + P^{22} v_2^2 \leqslant \left(\frac{1}{2\pi}\right)^2 \right\}$$

from (15a) and (22). In general $\mathbf{D}$ and $\lambda \cdot \mathbf{D}$ are ellipses. So we obtain $\mathrm{vol}_2(\mathbf{D}) = 1/(4\pi\sqrt{P^{11} \cdot P^{22}})$ if we consider the fact that the area $\mathrm{vol}_2(\mathcal{F}(\Gamma^*))$ of the fundamental domain $\mathcal{F}(\Gamma^*)$ ($\mathcal{F}(\Gamma^*)$ spanned by $\mathfrak{b}^1$ and $\mathfrak{b}^2$) is fixed to be equal to 1 (see (18)). The asymptotical expansion of $N(\lambda)$ for all P according to (20) is

$$N(\lambda) = \frac{1}{8\pi\sqrt{P^{11} \cdot P^{22}}} \lambda^2 + O(\lambda^{2/3}) .$$

If we investigate the important case that the metric fundamental tensor g^{hk} from (3b) defines the coefficients P^{hk} of P $P^{hk} := g^{hk}$ or, vice versa, P^{hk} delivers the metric in $\mathbf{E}^2$, we obtain $P = \partial_1^2 + \frac{1}{4}\partial_2^2 + \dots$ and

$$N(\lambda) = \frac{1}{4\pi} \lambda^2 + O(\lambda^{2/3}) .$$

Then $\mathbf{D}$ and $\lambda \cdot \mathbf{D}$ are circles.

Exact estimation of $N(\lambda)$ by counting the principal classes in $\lambda \cdot \mathbf{D}$ for small values of λ

This estimation could be carried out in general as in the case of $P^{hk} = g^{hk}$, i.e. $P = \partial_1^2 + \frac{1}{4}\partial_2^2$ (for the sake of simplicity, let $P^2 = 0$). Then $\lambda \cdot \mathbf{D}$ is the circle $v_1^2 + \frac{1}{4}v_2^2 \leqslant (\lambda/2\pi)^2$ with respect to the base $\{0; \mathfrak{b}^1, \mathfrak{b}^2\}$ or $(x^1)^2 + (x^2)^2 \leqslant (\lambda/2\pi)^2$ with respect to $\{0; \mathfrak{e}_1, \mathfrak{e}_2\}$. In fig. 1 we count the principal classes $\mathfrak{h}_1$, $\mathfrak{h}_2$ which are contained in $\lambda \cdot \mathbf{D}$ and on the circumference of $\lambda \cdot \mathbf{D}$ (in general $\lambda \cdot \mathbf{D}$ are ellipses). The result $N(\lambda)$ of the counting is represented in table 1 and fig. 2. Naturally $N(\lambda)$ is a step function. In table 1 the function values $N(\lambda)$ are given just at the jump discontinuities $\lambda = 2\pi \cdot R$, where $R = \sqrt{(x^1)^2 + (x^2)^2}$ is the radius of $\lambda \cdot \mathbf{D}$ but here we understand (x^1, x^2) as a lattice point $(x^1, x^2) \in \mathfrak{h}_i \subset \Gamma^*$. The magnitude of the discontinuity of N on λ is equal to the number of principal classes on the periphery of $\lambda \cdot \mathbf{D}$. Figure 2 and table 1 represent also the comparison between the exact step function $N(\lambda)$ and its asymptotic estimation $N(\lambda) \sim \lambda^2/4\pi$.

(b) The group $\mathfrak{G} = \Delta^2_{p31m}$

As for $\mathfrak{G} = \Delta^2_{pg}$ in section 2.2(a), we first estimate the Δ^2_{p31m}-invariant differential operators P by means of the invariance condition (19) with respect to $\sigma = \alpha, \beta, \gamma, \delta, \zeta \in \mathfrak{L}$. Easy algebraic calculations deliver all invariant operators,

$$P = c\left(\frac{\partial^2}{\partial v^{1^2}} + \frac{\partial^2}{\partial v^1 \partial v^2} + \frac{\partial^2}{\partial v^{2^2}}\right), \quad c>0, \quad \mathfrak{v} = v^h \mathfrak{b}_h. \tag{25}$$

The assigned characteristic polynom is

$$P(\mathfrak{v}) = -c(v_1^2 + v_1 v_2 + v_2^2), \quad c>0, \quad \mathfrak{v} = v_h \mathfrak{b}^h, \tag{26}$$

and therefore the P-norm of $\mathfrak{v}$ is

$$\|\mathfrak{v}\| = \sqrt{c}(v_1^2 + v_1 v_2 + v_2^2)^{1/2}. \tag{27}$$

For the above P we solve the Δ^2_{p31m}-automorphic eigenvalue problem $P[\psi] + \mu\psi = 0$ according to (12), (13) and (26). Of course here for the principal classes $\mathfrak{h}$ we must take $\mathfrak{h}_1 = \mathfrak{k}_1$, $\mathfrak{h}_3^{\pm} = \mathfrak{k}_3^{\pm}$, $\mathfrak{h}_6 = \mathfrak{k}_6$ from (8). To establish formula (12) for $\mathfrak{h} = \mathfrak{h}_1, \mathfrak{h}_3^{\pm}, \mathfrak{h}_6$ we must first consider

$$\mathfrak{R}(\mathfrak{u}_1) = \begin{cases} \mathfrak{L} \\ \{e, \beta\}, \\ \{e\} \end{cases} \quad \operatorname{rep}(\mathfrak{L}/\mathfrak{R}(\mathfrak{u}_1))_{\mathrm{L}} = \begin{cases} \{e\} & \mathfrak{u}_1 \in \mathfrak{h}_1, \\ \{e, \alpha, \gamma\} \quad \text{if} & \mathfrak{u}_1 \in \mathfrak{h}_3^{\pm}, \\ \mathfrak{L} & \mathfrak{u}_1 \in \mathfrak{h}_6. \end{cases}$$

If we consider that for $\mathfrak{u} \in \Gamma^*$ and for $\mathfrak{s} = \mathfrak{a}, \mathfrak{b}, \mathfrak{g}, \mathfrak{d}, \mathfrak{z} \equiv 0 \bmod \mathfrak{t}$ (see section 1.5(b)) the relation $\varphi_{\mathfrak{u}}(\mathfrak{s}) = 1$ is true, we obtain

$$\psi_{\mathfrak{h}_1}(\mathfrak{x}) = 1, \quad \mu_{\mathfrak{h}_1} = 0;$$

$$\begin{aligned} \psi_{\mathfrak{h}_3^{\pm}}(\mathfrak{x}) &= \frac{1}{\sqrt{3}}(\varphi_{\pm u(\mathfrak{b}^1+\mathfrak{b}^2)}(\mathfrak{x}) + \varphi_{\pm u(\mathfrak{b}^1-2\mathfrak{b}^2)}(\mathfrak{x}) + \varphi_{\pm u(-2\mathfrak{b}^1+\mathfrak{b}^2)}(\mathfrak{x})) \\ &= \frac{1}{\sqrt{3}}(\varphi_{\mathfrak{u}}(\mathfrak{x}) + \varphi_{\mathfrak{u}}(\alpha\mathfrak{x}) + \varphi_{\mathfrak{u}}(\gamma\mathfrak{x})), \end{aligned}$$

$$\mu_{\mathfrak{h}_3^{\pm}} = 12c(\pi u)^2,$$

where

$$\mathfrak{u} = \pm u(\mathfrak{b}^1 + \mathfrak{b}^2) \in \mathfrak{h}_3^{\pm}, \quad 0<u\in\mathbf{Z};$$

$$\begin{aligned} \psi_{\mathfrak{h}_6}(\mathfrak{x}) = {} & \frac{1}{\sqrt{6}}(\varphi_{u_i\mathfrak{b}^i}(\mathfrak{x}) + \varphi_{u_1\mathfrak{b}^1-(u_1+u_2)\mathfrak{b}^2}(\mathfrak{x}) + \varphi_{u_2\mathfrak{b}^1+u_1\mathfrak{b}^2}(\mathfrak{x}) \\ & + \varphi_{u_2\mathfrak{b}^1-(u_1+u_2)\mathfrak{b}^2}(\mathfrak{x}) + \varphi_{-(u_1+u_2)\mathfrak{b}^1+u_1\mathfrak{b}^2}(\mathfrak{x}) \\ & + \varphi_{-(u_1+u_2)\mathfrak{b}^1+u_2\mathfrak{b}^2}(\mathfrak{x}) \\ = {} & \frac{1}{\sqrt{6}}\sum_{\sigma\in\mathfrak{L}}\varphi_{\mathfrak{u}}(\sigma\mathfrak{x}), \quad \mu_{\mathfrak{h}_6} = (2\pi)^2 c(u_1^2 + u_1 u_2 + u_2^2), \end{aligned}$$

where $\mathfrak{u} = u_i \mathfrak{b}^i \in \mathfrak{h}_3$.

If $\mathfrak{h}_1$, $\mathfrak{h}_3^\pm$ and $\mathfrak{h}_6$ run through the set $\mathfrak{H}$ of all principal classes of Δ^2_{p31m} we obtain all eigenvalues $\mu_{\mathfrak{h}_i}$ and eigenfunctions $\psi_{\mathfrak{h}_i}(\mathfrak{x})$ of the Δ^2_{p31m}-automorphic eigenvalue problem (11).

The number $N(\lambda)$ of eigenvalues

We consider the asymptotic estimation of $N(\lambda)$ in (17). Relative to $\mathfrak{G} = \Delta^2_{p31m}$ comes out $n = 2$, $r = 6$; $\mathfrak{L}_1 = \{\alpha, \beta, \zeta\}$ and $\delta_\alpha = \delta_\beta = \delta_\zeta = 1$ because of $\mathfrak{a}, \mathfrak{b}, \mathfrak{z} \equiv 0 \bmod \mathfrak{t}$. To ascertain $\mathfrak{L}_1$ and $\mathrm{vol}_1(\mathbf{D} \cap \mathfrak{V}^*(\sigma))$ we have to establish the vector spaces $\mathfrak{V}^*(\sigma)$ for $\sigma = e, \alpha, \beta, \gamma, \delta, \zeta$:

$$\mathfrak{V}^*(\alpha) = \{\mathfrak{v} = v(-2\mathfrak{b}^1 + \mathfrak{b}^2) | v \in \mathbf{R}\}, \quad \dim \mathfrak{V}^*(\alpha) = 1,$$

$$\mathfrak{V}^*(\beta) = \{\mathfrak{v} = v(\mathfrak{b}^1 + \mathfrak{b}^2) | v \in \mathbf{R}\}, \quad \dim \mathfrak{V}^*(\beta) = 1,$$

$$\mathfrak{V}^*(\gamma) = \mathfrak{V}^*(\delta) = \{0\}, \quad \dim \mathfrak{V}^*(\gamma) = \dim \mathfrak{V}^*(\delta) = 0,$$

$$\mathfrak{V}^*(\zeta) = \{\mathfrak{v} = v(\mathfrak{b}^1 - 2\mathfrak{b}^2) | v \in \mathbf{R}\}, \quad \dim \mathfrak{V}^*(\zeta) = 1.$$

The equation of the circle $\mathbf{D}$ relative to the base $\{0; \mathfrak{e}_1, \mathfrak{e}_2\}$ is $(x^1)^2 + (x^2)^2 = 1/(3c\pi^2)$; $2R = 2/(\sqrt{3c}\pi)$ is the diameter of $\mathbf{D}$ and therefore $\mathrm{vol}_1(\mathbf{D} \cap \mathfrak{V}^*(\sigma)) = 2/(\sqrt{3c}\pi)$ for $\sigma = \alpha, \beta, \zeta$. So we obtain with regard to (18)

$$\begin{aligned} N(\lambda) &= \tfrac{1}{6}\mathrm{vol}_2(\mathbf{D}) \cdot \lambda^2 \\ &\quad + \tfrac{1}{6}(\mathrm{vol}_1(\mathbf{D} \cap \mathfrak{V}^*(\alpha)) + \mathrm{vol}_1(\mathbf{D} \cap \mathfrak{V}^*(\beta)) + \mathrm{vol}_1(\mathbf{D} \cap \mathfrak{V}^*(\zeta))) \cdot \lambda \\ &\quad + O(\lambda^{2/3}) \\ &= \frac{1}{12\sqrt{3}\pi c}\lambda^2 + \frac{1}{2\sqrt{3c}\pi}\lambda + O(\lambda^{2/3}), \quad c > 0. \end{aligned} \tag{28}$$

REMARK 5

Because of (18) the fundamental domain $\mathfrak{F}(\mathfrak{e}_1 \times \mathfrak{e}_2)$ (which is spanned by $\mathfrak{e}_1$, $\mathfrak{e}_2$) is equal to $\sqrt{3}/2$. This factor must be considered for the calculation of

$$\mathrm{vol}_2(\mathbf{D}) = \frac{1}{3\pi c}\frac{\sqrt{3}}{2}.$$

Exact estimation of $N(\lambda)$ by counting the principal classes in $\lambda \cdot \mathbf{D}$ for small values of λ

As in example $\mathfrak{G} = \Delta^2_{pg}$, fig. 1, we now count the principal classes $\mathfrak{h}_1$, $\mathfrak{h}_3^\pm$, $\mathfrak{h}_6$ from $\mathfrak{G} = \Delta^2_{p31m}$ in the circle $\lambda \cdot \mathbf{D}$: $(x^1)^2 + (x^2)^2 \leqslant R^2$ with $R = \lambda/(\sqrt{3c}\pi)$ by means of fig. 3 for $c = 4/3$. The result is shown in fig. 4 and table 2. Important is the following remark about the structure of $N(\lambda)$ in (17) or (28).

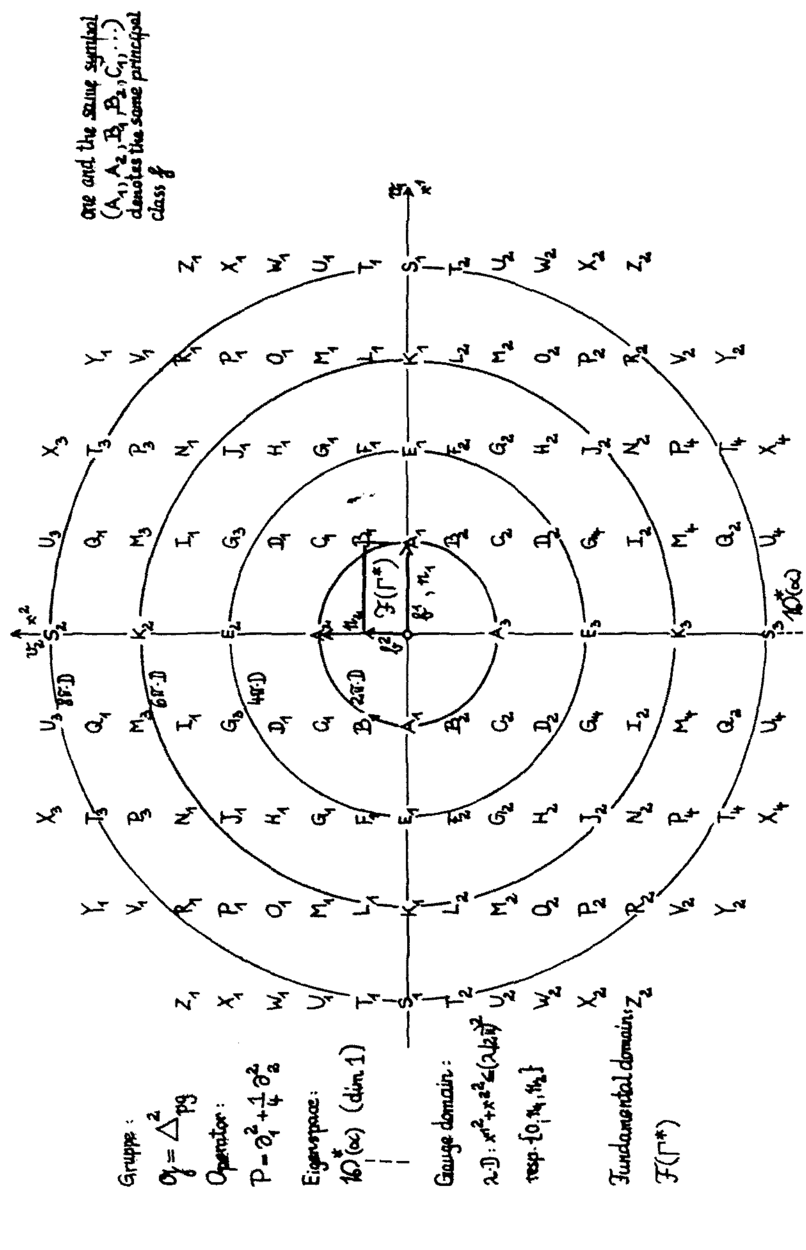

Gruppe:
Operator:
Eigenspace:
Gauge domain:
Fundamental domain:
are and the same symbol (A1, A2, B1, B2, C1, ...) denotes the same principal class

Fig. 1.

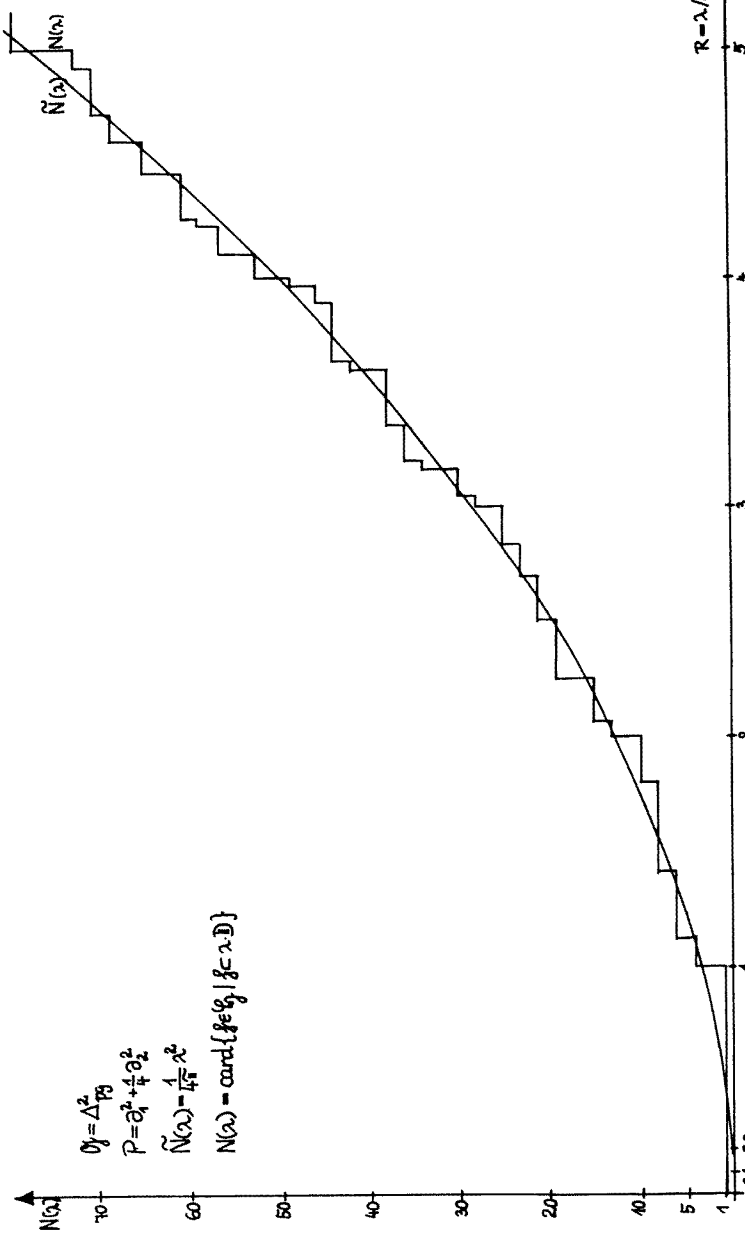


Fig. 2.

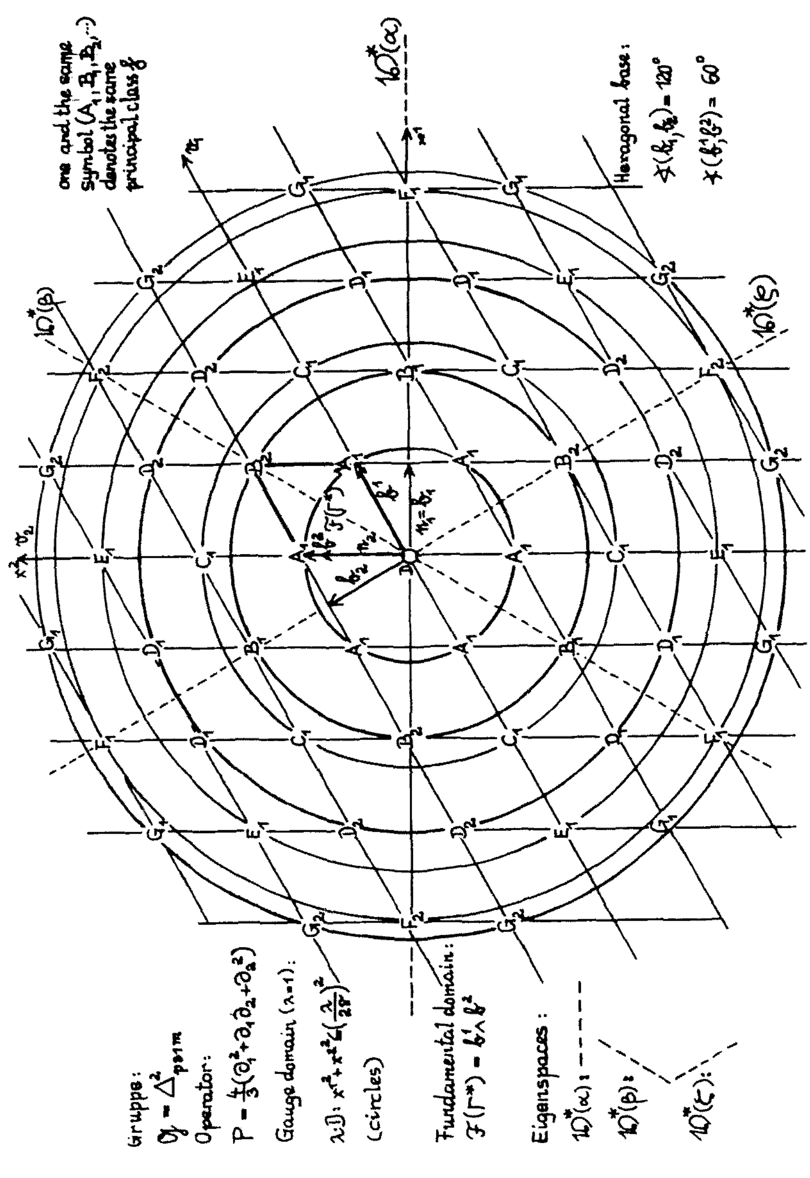

Gruppe:
Operator:
Gauge domain (λ=1):
(circles)
Fundamental domain:
Eigenspaces:
Hexagonal base:
one and the same symbol denotes the same principal class

Fig. 3.

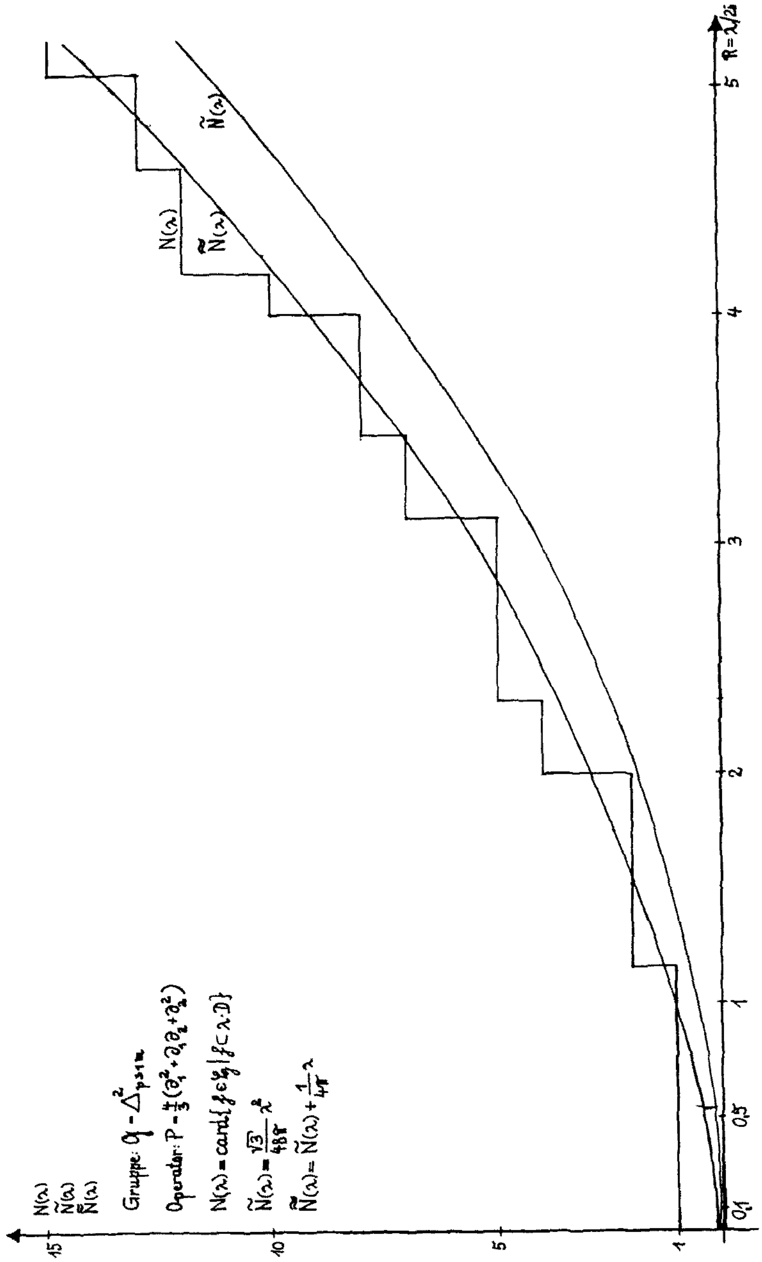

N(λ)
Ñ(λ)
$\tilde{\tilde{N}}(\lambda)$
Gruppe: $\mathcal{G} = \Delta^2_{p31m}$
Operator: $P = \frac{4}{3}(\partial_1^2 + \partial_1\partial_2 + \partial_2^2)$
$N(\lambda) = \text{card}\{\mathcal{f} \in \mathcal{V}_{\mathcal{G}} \mid \mathcal{f} \subset \lambda \cdot D\}$
$\tilde{N}(\lambda) = \frac{\sqrt{3}}{48\pi}\lambda^2$
$\tilde{\tilde{N}}(\lambda) = \tilde{N}(\lambda) + \frac{1}{4\pi}\lambda$
15
10
5
1
0,1
0,5
1
2
3
4
5
$R = \lambda/2\pi$
N(λ)
$\tilde{\tilde{N}}(\lambda)$
Ñ(λ)

Fig. 4.

Table 1

(x^1, x^2)	(0, 0)	(1, 0)	(1, 1/2)	(1, 1)	(1, 3/2)	(2, 0)	(2, 1/2)	(2, 1)	(2, 3/2)	(1, 5/2)	(2, 2)	(3, 0)	(3, 1/2)	(3, 1)	(2, 5/2)
$R = \sqrt{x^{1^2} + x^{2^2}}$	0	1	1.12	1.41	1.80	2	2.06	2.24	2.5	2.69	2.83	3	3.04	3.16	3.20
$\lambda = 2\pi R$	0	2π	7.02	8.89	11.33	4π	12.95	14.05	15.71	16.92	17.78	6π	19.11	19.87	20.12
$N(\lambda)$	1	4	6	8	10	13	15	19	21	23	25	28	30	34	36
$\bar{N}(\lambda) = \lambda^2/4\pi$	0	π	3.92	6.29	10.22	4π	13.35	15.71	19.64	22.78	25.16	9π	29.06	31.42	32.21
(x^1, x^2)	(3, 3/2)	(3, 2)	(1, 7/2)	(3, 5/2)	(4, 0)	(4, 1/2)	(4, 1)	(3, 3)	(4, 3/2)	(4, 2)	(3, 7/2)	(4, 5/2)	(2, 9/2)	(4, 3)	
$R = \sqrt{x^{1^2} + x^{2^2}}$	3.35	3.61	3.64	3.91	4	4.03	4.12	4.24	4.27	4.47	4.61	4.72	4.92	5	
$\lambda = 2\pi R$	21.07	22.65	22.87	24.54	8π	25.33	25.91	26.66	26.84	28.10	28.96	29.64	30.94	10π	
$N(\lambda)$	38	42	44	46	49	53	57	59	61	65	69	71	73	80	
$\bar{N}(\lambda) = \lambda^2/4\pi$	35.33	40.83	41.62	47.92	16π	51.06	53.42	56.56	57.33	62.84	66.74	69.91	76.18	25π	

Table 2

(x^1, x^2)	(0,0)	$(1, 1/\sqrt{3})$	(2,0)	$(2, 2/\sqrt{3})$	$(3, 1/\sqrt{3})$	$(3, 3/\sqrt{3})$	(4,0)	$(4, 2/\sqrt{3})$	$(4, 4/\sqrt{3})$	$(5, 1/\sqrt{3})$
$R = \sqrt{x^{1^2} + x^{2^2}}$	0	1.15	2	2.31	3.10	3.46	4	4.16	4.62	5.03
$\lambda = 2\pi R$	0	7.26	4π	14.51	19.20	21.77	8π	26.16	29.02	31.62
$N(\lambda)$	1	2	4	5	7	8	10	12	13	15
$\tilde{N}(\lambda)$	0	0.60	1.81	2.42	4.23	5.44	7.26	7.86	9.67	11.49
$\tilde{\tilde{N}}(\lambda)$	0	1.18	2.81	3.57	5.76	7.17	9.26	9.94	11.98	14.00

$\tilde{N}(\lambda) = \frac{\sqrt{3}}{48\pi}\lambda^2$, $\tilde{\tilde{N}}(\lambda) = \tilde{N}(\lambda) + \frac{1}{4\pi}\lambda$

Table 3

e	α	β	γ	δ	ζ
α	e	γ	β	ζ	δ
β	δ	e	ζ	α	γ
γ	ζ	α	δ	e	β
δ	β	ζ	e	γ	α
ζ	γ	δ	α	β	e

REMARK 6

The asymptotic of $N(\lambda)$ is $N(\lambda) \sim c_0 \cdot \lambda^n + c_1 \cdot \lambda^{n-1}$; $c_0 \cdot \lambda^n$ is said to be the principal part and $c_1 \cdot \lambda^{n-1}$ the second part of $N(\lambda)$. What is new about the asymptotic of $N(\lambda)$ from (17) is just the fact that $N(\lambda)$ contains not only a principal part but also a second part.

So we are able to give a comparison of exactitude between $N(\lambda)$, $\tilde{N}(\lambda) := c_0 \cdot \lambda^n$ and $\tilde{\tilde{N}}(\lambda) := c_0 \cdot \lambda^n + c_1 \cdot \lambda^{n-1}$. For $\mathfrak{G} = \Delta^2_{p31m}$ this is most impressively shown in fig. 4.

3. Concluding remarks

Already one year after the exposition about the black-body radiation which was given by H.A. Schwarz during the course of the 1909 annual meeting of the German Physical Society in Königsberg, H. Weyl reflected on this important development in a paper about the asymptotic behaviour of $N(\lambda)$ (see, e.g., [17], later [18], etc.). Weyl's asymptotic estimations extend only up to the so-called principal term $c_0 \cdot \lambda^n$: $N(\lambda) \sim c_0 \cdot \lambda^n$ (λ: frequency bound, c_0: constant, n: dimension of the space). But already the conjecture of Weyl/Pòlya does concern the presumption that there exists also a "second term" $c_1 \cdot \lambda^{n-1}$ with $N(\lambda) \sim c_0 \cdot \lambda^n + c_1 \cdot \lambda^{n-1}$. Just this conjecture is certified by formula (17) for invariant operators (with respect to crystallographic groups or more general properly discontinuous groups).

The knowledge of the second part $c_1 \cdot \lambda^{n-1}$ improves the asymptotic of $N(\lambda)$ essentially.

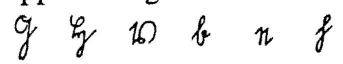
We should also think about the theory of quantum chaos where oscillatory corrections to Weyl-type terms are associated with periodic orbits (closed geodesic in manifolds) or to the density of the orbits of crystallographic groups [14].

Glossary to figures 1–4

The Fraktur letters within the text or in formulas:

$\mathfrak{G}$ $\mathfrak{H}$ $\mathfrak{W}$ $\mathfrak{b}$ $\mathfrak{e}$ $\mathfrak{h}$

appear in figures 1–4 in the old-fashioned style of German hand-writing, i.e. as:



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