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Fourierovy–Weylovy transformace a jejich aplikace Fourier–Weyl Transforms and Their Applications

Summary

Symmetries of physical systems are essential for construction and mathematization of the related physical theories and models. The classical theory of Lie algebras and their Weyl groups establishes a connection between group theory and modern physics. Multivariate exponential functions associated to crystallographic root systems of complex simple Lie algebras and their corresponding affine Weyl groups constitute a standard segment of Lie theory and its application in mathematical physics. As signed sums of the multivariate exponential functions, the complex-valued Weyl orbit functions and real-valued Hartley orbit functions represent generalizations of the classical trigonometric functions. The set of multivariate generalizations of the cosine and sine functions is further enriched using the concept of sign homomorphisms. The Fourier–Weyl and Hartley–Weyl discrete transforms incorporate kernels of the Weyl and Hartley orbit functions, respectively, and are constructed on finite fragments of the Weyl group invariant lattices. The weight lattice Fourier-Weyl transforms are linked to the dual Kac-Walton formulas and to the Kac–Peterson matrices in conformal field theory. Subtraction of the weight and root lattice Hartley–Weyl transforms for the A_2 case generates the honeycomb lattice transforms that are applied to vibrations of the mechanical graphene model.

Souhrn

Symetrie fyzikálních systémů jsou zásadní pro konstrukci a matematizaci odpovídajících fyzikálních teorií a modelů. Klasická teorie Lieových algeber a jejich Weylových grup určuje spojení mezi teorií grup a moderní fyzikou. Exponenciální funkce více proměnných příslušející krystalografickým kořenovým systémům komplexních Lieových algeber a jejich afinních Wevlových grup tvoří standardní část Lieovy teorie a její aplikace v matematické fyzice. Vytvořeny jako sumy se znaménky exponenciálních funkcí více proměnných, komplexní Weylovy orbitové funkce a reálné Hartlevho orbitové funkce představují zobecnění klasických trigonometrických funkcí. Soubor zobecněných cosinů a sinů je dále obohacen užitím konceptu znaménkových homomorfismů. Fourierovy-Weylovy a Hartleyovy-Weylovy diskrétní transformace, obsahující Weylovy a Hartleyho orbitové funkce, jsou zkonstruovány na konečných fragmentech mříží, které jsou invariantní vůči Weylovým grupám. Fourierovy–Weylovy transformace na váhových mřížích jsou dány do souvislosti s duálními Kacovými–Weylovými formulemi a Kacovými– Petersonovými maticemi z konformní teorie pole. Odečtení Hartlevových-Weylových váhových a kořenových transformací algebry A_2 generuje transformace na plástvové mřížce, které jsou aplikovány na vibrace mechanického modelu grafénu.

Klíčová slova: Fourierova transformace, Weylova grupa, orbitové funkce, diskrétní ortogonalita

Keywords: Fourier transform, Weyl group, orbit functions, discrete orthogonality $% \mathcal{A}(\mathcal{A})$

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1 Introduction

Continuous and discrete symmetries of physical systems are fundamental for construction and mathematization of the related physical theories and models. Group theory forms a central part of mathematical description and analysis of the inherent symmetries. The classical theory of Lie groups and Lie algebras establishes an essential connection between group theory and modern physics. Multivariate exponential functions associated to crystallographic root systems of complex simple Lie algebras and their corresponding affine Weyl groups constitute a standard segment of Lie theory and its application in mathematical physics [1, 13]. The Weyl orbit functions are embedded in conformal field theory [4] and appear implicitly in solid state physics [17].

The Weyl orbit functions represent multivariate generalizations of the classical trigonometric functions [1,13]. Symmetric sums of exponential functions, directly connected to multivariate versions of Chebyshev polynomials [1], are named *C*-functions in [15, 16] and serve as generalizations of the cosine function. Antisymmetric S-functions from the Weyl character formula lead to generalizations of the sine function. Symmetry and antisymmetry properties of the C- and S-functions with respect to their inherent Weyl groups together with the translation invariance by shifts from the dual root lattice permit restrictions of these functions to the fundamental domains of their affine Weyl groups [13]. The fundamental domains in the form of the Weyl alcoves constitute generalizations of the one-dimensional interval as domain for the classical cosine and sine functions [13]. The dual root system and the dual affine Weyl group first appear in the description of the labels of the C- and S-functions and the corresponding fully explicit form of the dual weight-lattice Fourier-Weyl transforms [10]. The boundary behavior of the hybrid orbit functions with respect to both point and label domains results in the corresponding hybrid Fourier–Weyl transforms in [9].

Conformal field theories with the Lie group symmetry regularly utilize the antisymmetric Weyl orbit functions and their discrete weight lattice Fourier-Weyl transforms [4, 19]. A correspondence between the dual weight discretization of Weyl orbit functions and affine modular data associated with conformal field theories is developed in [11]. Products of the discretized orbit functions are analogous with truncations of tensor products which determine interactions in the conformal field models. A significant tool for description of the tensor products, which leads to an efficient algorithm for calculation of the fusion coefficients, is the Kac–Walton formula [4]. The generalization of the Kac-Walton formula for the dual weight lattice Fourier-Weyl transforms from [10] and the related Galois symmetries are developed in [11]. Three additional generalizations of the Kac–Peterson unitary and symmetric S-matrices resulting from the symmetric and hybrid Weyl orbit functions are constructed in [12]. Apart from conformal field theory, the Fourier–Weyl and Hartley–Weyl transforms found also direct applications to eigenvibrations of mechanical models in solid state physics.

The 2D and 3D mechanical vibration models based on the Fourier–Weyl transforms retain Weyl group symmetries and determine vibrations of the Weyl group invariant lattices. General cases of the mechanical vibration models in solid state physics constitute fundamental stepping stones for their quantum field versions [5]. Dispersion relations of these models are systematically derived in solid state physics assuming solutions in exponential form while imposing periodic Born-von Kármán boundary conditions. The Hartley orbit functions represent multidimensional generalizations of the cosine and sine standing waves solutions of the one-dimensional beaded string subjected to Neumann and Dirichlet conditions, respectively. The spectral analysis of initial conditions provided by the Hartley–Weyl transforms enables calculation of time evolving exact solutions of the mechanical models. A special case of such mechanical models, the mechanical graphene model [3], is currently intensively investigated [14] in connection with the relevant graphene material [5]. Transversal eigenvibrations of the equilateral triangular sheets of the mechanical graphene and the wave functions of the quantum particle on the same triangular honeycomb point set [17] are determined by the honeycomb Hartley and Weyl orbit functions from [7].

2 Affine Weyl groups

To each complex simple Lie algebra from the four infinite series and the five exceptional cases corresponds the set of vectors $\Delta = \{\alpha_1, \ldots, \alpha_n\} \subset \mathbb{R}^n$, that are called simple roots [1]. Each set of simple roots Δ constitutes a non-orthogonal basis of the Euclidean space \mathbb{R}^n with the standard scalar product $\langle \cdot, \cdot \rangle$. There are two types of the sets of simple roots Δ . The first type of Δ consists of the roots of one length only and comprises the series A_n $(n \geq 1)$, D_n $(n \geq 4)$ and three special cases E_6, E_7, E_8 . The second type contains roots with two different lengths and is represented by the series B_n $(n \geq 3)$, C_n $(n \geq 2)$ and two exceptional cases F_4, G_2 . For the cases of Δ with two different root-lengths, the set Δ is disjointly decomposed into a set Δ_s of short simple roots and a set Δ_l of long simple roots,

$$\Delta = \Delta_s \cup \Delta_l. \tag{1}$$

Every simple root $\alpha_i \in \Delta$ induces a reflection r_i and the set of reflections $r_i, i \in \{1, \ldots, n\}$ generates a finite Weyl group W of orthogonal operators. Action of the Weyl group W on the set Δ generates the root system Π , $\Pi = W\Delta$. The current notion of the root system coincides with a more general notion of root systems from the theory of Coxeter groups, the root systems corresponding to the complex simple Lie algebras are called irreducible and crystallographic [13].

The highest root $\xi \in \Pi$ is expressed as a linear combination of the simple roots $\xi = m_1 \alpha_1 + \cdots + m_n \alpha_n$, with non-negative integer coefficients

 $m_1, \ldots, m_n \in \mathbb{N}$. The numbers $q_1, \ldots, q_n \in \mathbb{N}$ associated to the marks via relation

$$q_i = \frac{m_i \langle \alpha_i, \alpha_i \rangle}{2}, \quad i \in \{1, \dots, n\},$$
(2)

are called the comarks. A circle inversion of simple roots $\alpha_i \in \Delta$, $\alpha_i^{\vee} = 2\alpha_i/\langle \alpha_i, \alpha_i \rangle$, leads to a set of the vectors $\Delta^{\vee} = \{\alpha_1^{\vee}, \ldots, \alpha_n^{\vee}\}$ that is also a set of simple roots of some complex simple Lie algebra. The set Δ^{\vee} generates the entire dual root system via action of the Weyl group, $\Pi^{\vee} = W \Delta^{\vee}$.

There are four classical Weyl group invariant lattices: the root lattice, the dual weight lattice, the dual root lattice and the weight lattice. The root lattice Q is the integer span of the set of simple roots Δ ,

$$Q = \mathbb{Z}\alpha_1 + \dots + \mathbb{Z}\alpha_n.$$

The dual weight lattice P^{\vee} is \mathbb{Z} -dual to the root lattice Q,

$$P^{\vee} = \mathbb{Z}\omega_1^{\vee} + \dots + \mathbb{Z}\omega_n^{\vee},$$

where the vectors ω_i^{\vee} are called the dual fundamental weights and are determined by the duality formula, $\langle \omega_i^{\vee}, \alpha_j \rangle = \delta_{ij}$. The dual root lattice Q^{\vee} is the integer span of the set of dual simple roots Δ^{\vee} ,

$$Q^{\vee} = \mathbb{Z}\alpha_1^{\vee} + \dots + \mathbb{Z}\alpha_n^{\vee}.$$

The weight lattice P is \mathbb{Z} -dual to the dual root lattice Q^{\vee} ,

$$P = \mathbb{Z}\omega_1 + \dots + \mathbb{Z}\omega_n,\tag{3}$$

where the vectors ω_i are called the fundamental weights and are determined by the duality formula, $\langle \omega_i, \alpha_j^{\vee} \rangle = \delta_{ij}$. The cone of the dominant weights is given as

$$P_{+} = \mathbb{Z}^{\geq 0}\omega_{1} + \dots + \mathbb{Z}^{\geq 0}\omega_{n}.$$
(4)

The Gram determinant d of the α^{\vee} -basis determines the order of the quotient group P/Q^{\vee} ,

$$d = \det\langle \alpha_i^{\vee}, \, \alpha_j^{\vee} \rangle = |P/Q^{\vee}|. \tag{5}$$

The group of shifts Q^{\vee} generates the affine Weyl group $W^{\rm aff}$ expressed as the semidirect product,

$$W^{\text{aff}} = Q^{\vee} \rtimes W,\tag{6}$$

that induces the retraction homomorphism $\psi: W^{\text{aff}} \to W$. The group of shifts Q generates the dual affine Weyl group \widehat{W}^{aff} expressed as the semidirect product,

$$\widehat{W}^{\text{aff}} = Q \rtimes W,\tag{7}$$

that induces the dual retraction homomorphism $\widehat{\psi}: \widehat{W}^{\mathrm{aff}} \to W$.

The augmented dual affine Weyl group $\widehat{W}_M^{\text{aff}}$ is defined for any scaling factor $M \in \mathbb{N}$ by relation

$$\widehat{W}_{M}^{\text{aff}} = MQ \rtimes W.$$
(8)

Any homomorphism $\sigma: W \mapsto \{\pm 1\}$ is called a sign homomorphism [9]. The identity 1 and the determinant σ^e sign homomorphisms, which exist for all Weyl groups W, are given on the generating reflections $r_i, \alpha_i \in \Delta$ as

$$\begin{aligned} \mathbf{1}(r_i) &= 1, \\ \sigma^e(r_i) &= -1. \end{aligned}$$

For the root systems with two lengths of roots, the short and long sign homomorphisms σ^s and σ^l are defined via decomposition (1) as

$$\sigma^{s}(r_{i}) = \begin{cases} -1, & \alpha_{i} \in \Delta_{s}, \\ 1, & \alpha_{i} \in \Delta_{l}, \end{cases}$$
$$\sigma^{l}(r_{i}) = \begin{cases} -1, & \alpha_{i} \in \Delta_{l}, \\ 1, & \alpha_{i} \in \Delta_{s}. \end{cases}$$

Defining the product \cdot of the sign homomorphisms pointwise [6], the resulting two-element and four-element abelian groups are isomorphic to \mathbb{Z}_2 and the Klein four-group, respectively.

The fundamental domains F and F^{\vee} consist of exactly one point of each W^{aff} and \widehat{W}^{aff} -orbits, respectively. The order of the isotropy subgroup $\operatorname{Stab}_{W^{\text{aff}}}(a)$ of any point $a \in \mathbb{R}^n$, defines for any $M \in \mathbb{N}$ a counting function $h_M : \mathbb{R}^n \to \mathbb{N}$ and a counting function $\varepsilon : \mathbb{R}^n \to \mathbb{N}$ by

$$h_M(a) = \left| \text{Stab}_{W^{\text{aff}}} \left(\frac{a}{M} \right) \right|, \quad \varepsilon(a) = \frac{|W|}{h_1(a)}. \tag{9}$$

The signed fundamental domain $F^{\sigma} \subset F$ is given as

$$F^{\sigma} = \left\{ a \in F \mid \sigma \circ \psi \left(\mathrm{Stab}_{W^{\mathrm{aff}}}(a) \right) = \{1\} \right\}$$

and the signed dual fundamental domain $F^{\sigma \vee} \subset F^{\vee}$ is given as

$$F^{\sigma \vee} = \left\{ a \in F^{\vee} \, \big| \, \sigma \circ \widehat{\psi} \left(\mathrm{Stab}_{\widehat{W}^{\mathrm{aff}}}(a) \right) = \{1\} \right\}.$$
(10)

3 Fourier–Weyl Transforms

The first major contribution of the author to the field of multivariate discrete Fourier transforms is presented in paper [10], where the two standard cases of discrete dual weight lattice Fourier–Weyl transforms of C–functions and S–functions are developed. These two basic transforms are generalized to all four sign homomorphisms in [9]. The Fourier-Weyl weight lattice transform and its link to the Kac–Peterson matrices from conformal field theory is developed in [12].

Two families of complex orbit functions $\varphi_b^{\sigma} : \mathbb{R}^n \to \mathbb{C}$ for any root system together with two additional families for the systems with two root-lengths are labeled by the labels $b \in \mathbb{R}^n$ and determined by the sign homomorphisms σ via signed symmetrization of exponential functions over the Weyl group W,

$$\varphi_b^{\sigma}(a) = \sum_{w \in W} \sigma(w) \, e^{2\pi i \langle wb, a \rangle}, \quad a \in \mathbb{R}^n.$$
(11)

Using the Hartley kernel functions [2] of the form $\cos a = \cos a + \sin a$, the real-valued Hartley orbit functions, introduced in [6–8], are given by

$$\zeta_b^{\sigma}(a) = \sum_{w \in W} \sigma(w) \cos 2\pi \langle wb, a \rangle, \quad a \in \mathbb{R}^n.$$
(12)

For any $w^{\rm aff}\in W^{\rm aff}$ and $a\in\mathbb{R}^n$ the argument symmetry of Weyl orbit functions is of the form

$$\varphi_b^{\sigma}(w^{\text{aff}}a) = \sigma \circ \psi(w^{\text{aff}}) \cdot \varphi_b^{\sigma}(a).$$
(13)

Besides the argument symmetry (13) of the four types of orbit functions φ_b^{σ} , valid for any labels $b \in P$, a different type of label symmetry is induced by restricting the points to the refined weight lattice. For a point $a \in \frac{1}{M}P$, $M \in \mathbb{N}$ together with any $w^{\text{aff}} \in W^{\text{aff}}$ and $b \in \mathbb{R}^n$, the label symmetry of orbit functions is of the form

$$\varphi^{\sigma}_{Mw^{\mathrm{aff}}\left(\frac{b}{M}\right)}(a) = \sigma \circ \psi(w^{\mathrm{aff}}) \cdot \varphi^{\sigma}_{b}(a).$$
(14)

Discrete values of both points $a \in \frac{1}{M}P$ and labels $b \in P$ of the orbit functions $\varphi_b^{\sigma}(a)$ are due to the argument symmetries restricted to the set of points $F_{P,M}^{\sigma}$,

$$F_{P,M}^{\sigma} = \frac{1}{M} P \cap F^{\sigma}, \tag{15}$$

and due to the label symmetries restricted to the set of labels $\Lambda_{P,M}^{\sigma}$,

$$\Lambda^{\sigma}_{P,M} = P \cap MF^{\sigma}.$$
 (16)

Relation (38) in [12] states that the cardinalities of the sets of labels and the sets of points coincide for each case,

$$|\Lambda_{P,M}^{\sigma}| = |F_{P,M}^{\sigma}|.$$

The vector space $\mathcal{F}_{P,M}^{\sigma}$ of complex functions $f: F_{P,M}^{\sigma} \to \mathbb{C}$ is equipped with a scalar product containing as weight the counting function (9). This weight lattice weighted scalar product is of the following form for any $f, g \in \mathcal{F}_{P,M}^{\sigma}$,

$$\langle f, g \rangle_{F_{P,M}^{\sigma}} = \sum_{a \in F_{P,M}^{\sigma}} \varepsilon(a) f(a) \overline{g(a)}.$$
 (17)

The orthogonality relations of weight lattice discretized orbit functions in the Hilbert space $\mathcal{F}_{P,M}^{\sigma}$ are summarized in Theorem 4.5 in [12]. Using the numbers (5) and counting functions (9), the orthogonality relations are for any labels $b, b' \in \Lambda_{P,M}^{\sigma}$ of the form

$$\langle \varphi_b^{\sigma}, \, \varphi_{b'}^{\sigma} \rangle_{F_{P,M}^{\sigma}} = d \, |W| \, M^n h_M(b) \, \delta_{b,b'}.$$
⁽¹⁸⁾

The forward weight lattice Fourier–Weyl transform calculates for any function $f \in \mathcal{F}_{P,M}^{\sigma}$ its spectral transform $\widehat{f} : \Lambda_{P,M}^{\sigma} \to \mathbb{C}$ by prescribing for any $b \in \Lambda_{P,M}^{\sigma}$ the value

$$\widehat{f}(b) = (d |W| M^n h_M(b))^{-1} \sum_{a \in F_{P,M}^{\sigma}} \varepsilon(a) f(a) \overline{\varphi_b^{\sigma}(a)}.$$
(19)

Due to the orthogonality relations (18), the backward weight lattice Fourier–Weyl transform returns the original function $f \in \mathcal{F}_{P,M}^{\sigma}$,

$$f(a) = \sum_{b \in \Lambda_{P,M}^{\sigma}} \widehat{f}(b) \varphi_b^{\sigma}(a), \quad a \in F_{P,M}^{\sigma}.$$
 (20)

The symmetric generalized Kac–Peterson matrices $S^{\sigma}_{\lambda,\mu}$, $\lambda, \mu \in \Lambda^{\sigma}_{P,k+q^{\sigma}}$, determined by their entries

$$S^{\sigma}_{\lambda,\mu} = \frac{i^{\frac{|\Pi|}{2}}\varphi^{\sigma}_{\lambda}\left(\frac{-\mu}{k+q^{\sigma}}\right)}{\sqrt{d(k+q^{\sigma})^{n}h_{k+q^{\sigma}}(\lambda)h_{k+q^{\sigma}}(\mu)}},$$
(21)

are unitary due to the orthogonality relations (18). Note that the relations $M = k + q^{\sigma}$, depending on the comarks (2) and their signed version given by relation (39) in [12], are substituted for the number M into (18). The matrices $S^{\sigma^e}_{\lambda,\mu}$ coincide with the standard Kac–Peterson S–matrices [4].

4 Modified Multiplication and Honeycomb Transforms

The contribution of the author to this field is demonstrated in paper [11], where the multiplication formulas and their modification, together with their Galois symmetry, are presented. The generalization of the discrete Fourier–Weyl and Hartley–Weyl transforms to honeycomb lattice, including the interpolation tests, is presented in [7].

Products of two types of orbit functions $\varphi^{\sigma}_{\lambda}$ and $\varphi^{\sigma'}_{\lambda'}$ are decomposed into the sums of orbit functions,

$$\varphi_{\lambda}^{\sigma} \varphi_{\lambda'}^{\sigma'} = \sum_{w \in W} \sigma'(w) \varphi_{\lambda+w\lambda'}^{\sigma \cdot \sigma'}, \qquad (22)$$

and products of orbit functions $\varphi_{\lambda}^{\sigma}(a)$ and $\varphi_{\lambda}^{\sigma'}(a')$ are decomposed as

$$\varphi_{\lambda}^{\sigma}(a)\,\varphi_{\lambda}^{\sigma'}(a') = \sum_{w\in W} \sigma'(w)\,\varphi_{\lambda}^{\sigma\cdot\sigma'}(a+wa').$$
⁽²³⁾

Besides the modified multiplication, these general product-to-sum decomposition formulas (22) and (23) are crucial for vibrations models with Neumann and Dirichlet boundary conditions.

The product decomposition formulas (22) from [11] of the C-functions are further expressed in the form,

$$\varphi_{\lambda}^{\mathbf{l}}(a)\,\varphi_{\mu}^{\mathbf{l}}(a) = \sum_{\nu\in P_{+}} \left\langle C|CC\right\rangle_{\lambda,\mu}^{\nu}\,\varphi_{\nu}^{\mathbf{l}}(a) \tag{24}$$

for all dominant weights $\lambda, \mu \in P_+$.

For the weights from the finite set of labels $\lambda, \mu \in P \cap MF^{1\vee}$ and the points from the refined dual weight point sets $a \in P^{\vee}/M \cap F^1$, the modified multiplication product decomposition formulas are of the form

$$\varphi_{\lambda}^{\mathbf{l}}(a) \varphi_{\mu}^{\mathbf{l}}(a) = \sum_{\nu \in P_{+}^{M}} {}_{M} \langle C | CC \rangle_{\lambda,\mu}^{\nu} \varphi_{\nu}^{\mathbf{l}}(a).$$
⁽²⁵⁾

The relations between the decomposition coefficients form the dual weight Kac–Walton formulas,

$${}_{M}\langle C|CC\rangle_{\lambda,\mu}^{\nu} = \sum_{w\in\widehat{W}_{M}^{\mathrm{aff}}} \langle C|CC\rangle_{\lambda,\mu}^{w\nu}.$$
(26)

A specific subtractive contruction of the honeycomb lattice in terms of the invariant root and weight lattices of the root system A_2 is considered in [7]. The point set $F_{Q,M}$ is the intersection of the fundamental domain F with the root lattice,

$$F_{Q,M} = \frac{1}{M}Q \cap F. \tag{27}$$

The honeycomb point set H_M is obtained from the point set $F_{P,M}^1$ by subtraction of $F_{Q,M}$,

$$H_M = F_{P,M}^1 \setminus F_{Q,M}.$$
 (28)

The weight set $\Lambda^1_{P,M}$ is of the following explicit form,

$$\Lambda_{P,M}^{\mathbf{1}} = \left\{ \lambda_1 \omega_1 + \lambda_2 \omega_2 \, | \, \lambda_0, \lambda_1, \lambda_2 \in \mathbb{Z}^{\geq 0}, \lambda_0 + \lambda_1 + \lambda_2 = M \right\},\,$$

and the points from $\Lambda^{1}_{P,M}$ are described by their Kac coordinates as

$$\lambda = [\lambda_0, \lambda_1, \lambda_2] \in \Lambda^1_{P,M}.$$
(29)

The action of the group $\Gamma_M = \{\mathbf{1}, \gamma_1, \gamma_2\}$ on a weight $[\lambda_0, \lambda_1, \lambda_2] \in \Lambda_{P,M}^1$ is the cyclic permutation group action on the coordinates $[\lambda_0, \lambda_1, \lambda_2]$,

$$\mathbf{1}[\lambda_0, \lambda_1, \lambda_2] = [\lambda_0, \lambda_1, \lambda_2],$$

$$\gamma_1[\lambda_0, \lambda_1, \lambda_2] = [\lambda_2, \lambda_0, \lambda_1],$$

$$\gamma_2[\lambda_0, \lambda_1, \lambda_2] = [\lambda_1, \lambda_2, \lambda_0].$$

The honeycomb weight set L_M is given explicitly as,

$$L_M = \left\{ [\lambda_0, \lambda_1, \lambda_2] \in \Lambda_{P,M}^1 \, | \, (\lambda_0 > \lambda_1, \lambda_0 > \lambda_2) \, \lor \, (\lambda_0 = \lambda_1 > \lambda_2) \right\}.$$

Propositions 3.3 and 3.4 in [7] relate the numbers of points and weights in the honeycomb sets as

$$|L_M| = \frac{1}{2} |H_M|.$$

The honeycomb weight sets L_6 and L_7 are depicted in Figure 3 in [7].

The extended C-functions are for a fixed $M \in \mathbb{N}$ labeled by $\lambda \in L_M$ and introduced by

$$\Phi_{\lambda}^{+}(x) = \mu_{\lambda}^{+,0}\varphi_{\lambda}^{\mathbf{1}}(x) + \mu_{\lambda}^{+,1}\varphi_{\gamma_{1}\lambda}^{\mathbf{1}}(x) + \mu_{\lambda}^{+,2}\varphi_{\gamma_{2}\lambda}^{\mathbf{1}}(x),
\Phi_{\lambda}^{-}(x) = \mu_{\lambda}^{-,0}\varphi_{\lambda}^{\mathbf{1}}(x) + \mu_{\lambda}^{-,1}\varphi_{\gamma_{1}\lambda}^{\mathbf{1}}(x) + \mu_{\lambda}^{-,2}\varphi_{\gamma_{2}\lambda}^{\mathbf{1}}(x),$$
(30)

where $\mu_{\lambda}^{\pm,0}, \mu_{\lambda}^{\pm,1}, \mu_{\lambda}^{\pm,2} \in \mathbb{C}$ denote for each $\lambda \in L_M$ six extension coefficients. The extension coefficients $\mu_{\lambda}^{\pm,k}$ given by

$$\mu_{\lambda}^{\pm,0} = \operatorname{Re}\left\{ (3+\sqrt{3}\,i)\varphi_{\lambda}^{\mathrm{I}}\left(\frac{\omega_{1}}{M}\right) \right\},$$

$$\mu_{\lambda}^{\pm,1} = 0,$$

$$\mu_{\lambda}^{\pm,2} = \operatorname{Re}\left\{ (3-\sqrt{3}\,i)\varphi_{\lambda}^{\mathrm{I}}\left(\frac{\omega_{1}}{M}\right) \right\} \pm 3\left|\varphi_{\lambda}^{\mathrm{I}}\left(\frac{\omega_{1}}{M}\right)\right|,$$
(31)

induce the normalization functions of the following form [7],

$$\mu^{\pm}(\lambda) = 9 \left| \varphi_{\lambda}^{\mathbf{1}} \left(\frac{\omega_{1}}{M} \right) \right| \left(2 \left| \varphi_{\lambda}^{\mathbf{1}} \left(\frac{\omega_{1}}{M} \right) \right| \pm \operatorname{Re} \left\{ (1 - \sqrt{3} \, i) \varphi_{\lambda}^{\mathbf{1}} \left(\frac{\omega_{1}}{M} \right) \right\} \right).$$
(32)

The vector space \mathcal{H}_M of complex functions $f : H_M \to \mathbb{C}$ is equipped with a scalar product containing the counting weight function (9). This honeycomb scalar product is of the following form for any $f, g \in \mathcal{H}_M$,

$$\langle f, g \rangle_{H_M} = \sum_{a \in H_M} \varepsilon(a) f(a) \overline{g(a)}.$$
 (33)

The orthogonality relations of honeycomb C-functions in the Hilbert space \mathcal{H}_M are summarized in Theorem 5.1 in [7]. Using the functions (9), the orthogonality relations are for any labels $\lambda, \lambda' \in L_M$ of the form

$$\langle \Phi_{\lambda}^{\pm}, \Phi_{\lambda'}^{\pm} \rangle_{H_M} = 12M^2 h_M(\lambda)\mu^{\pm}(\lambda)\delta_{\lambda\lambda'}, \qquad (34)$$

$$\langle \Phi_{\lambda}^{+}, \Phi_{\lambda'}^{-} \rangle_{H_M} = 0. \tag{35}$$

The forward honeycomb Fourier–Weyl C-transform calculates for any $f \in \mathcal{H}_M$ its spectral transforms $\hat{f}^{\pm} : L_M \to \mathbb{C}$ by prescribing for any $\lambda \in L_M$ the value

$$\widehat{f}^{\pm}(\lambda) = (12M^2 h_M(\lambda)\mu^{\pm}(\lambda))^{-1} \sum_{a \in H_M} \varepsilon(a) f(a) \overline{\Phi_{\lambda}^{\pm}(a)}.$$
(36)

The backward honeycomb Fourier–Weyl C-transform returns the original function $f \in \mathcal{H}_M$,

$$f(a) = \sum_{\lambda \in L_M} \left(\widehat{f}^+(\lambda) \Phi_{\lambda}^+(x) + \widehat{f}^-(\lambda) \Phi_{\lambda}^-(x) \right), \quad a \in H_M.$$
(37)

The honeycomb Hartley C-functions $\operatorname{Cah}_{\lambda}^{\pm}$ are straightforward modification of the honeycomb functions (30) that contain the Hartley orbit functions (12). The orthogonality relations of honeycomb Hartley C-functions are summarized in Theorems 5.2 and 5.3 in [7], respectively. The forward and backward honeycomb Fourier-Weyl and Hartley-Weyl transforms are of similar forms.



Figure 1: Lower transversal Hartley modes of the A_2 armchair mechanical graphene vibration model X_{λ}^{\pm} , $\lambda \in L_{30}$ satisfying Neumann boundary conditions. The full set of transversal modes of H_{30} contains $2|L_{30}| = 330$ elements.

5 Transversal Vibration Models

Application of the multiplication formulas and Fourier–Weyl transforms in solid state physics are demonstrated on the transversal vibration models of 2D lattices with Neumann boundary conditions. The transversal A_2 armchair mechanical graphene vibration model is for the case M = 6 depicted in Figure 2 from [7]. The dots of the point set H_M represent the points of masses m and the equilibrium distance between the two nearest points is denoted by R_0 . The honeycomb dots are linked with the nearest neighbours by the springs of spring constants κ and natural lengths l_0 . The parameter $\eta = l_0/R_0$, $\eta < 1$ measures the level of stretching of the system.

Transverse displacement scalar function is denoted as $\psi(a) \equiv \psi(a, t)$, $a \in H_M$, where t represents time. The linearized equation of motion for transversal displacement of any general point $a = a_1\omega_1 + a_2\omega_2 = (a_1, a_2) \in H_M$ is simplified via assuming a solution of the mode form

$$\psi(a,t) = X(a)\cos(\omega t + \varphi). \tag{38}$$

The extension coefficients (31) determine honeycomb Hartley C-functions of type II in [7], which are denoted by $\operatorname{Cah}_{\lambda}^{\pm}$, $\lambda \in L_M$. Type II honeycomb C-functions represent amplitudes of the transversal modes (38) of the model subjected to discretized Neumann boundary conditions,

$$X_{\lambda}^{\pm}(a) = \operatorname{Cah}_{\lambda}^{\pm}(a), \quad a \in H_M, \quad \lambda \in L_M.$$

Several lower transversal Hartley modes of the transversal A_2 armchair mechanical graphene vibration model are for Neumann and Dirichlet boundary conditions depicted in Figures 1 and 2, respectively.



Figure 2: Lower transversal Hartley modes of the A_2 armchair mechanical graphene vibration model satisfying Dirichlet boundary conditions. The full set of transversal modes of contains 270 elements.

The eigenfrequencies ω_{λ}^{\pm} corresponding to the modes X_{λ}^{\pm} , $\lambda \in L_M$ are given as

$$\omega_{\lambda}^{\pm} = \sqrt{\frac{\kappa(1-\eta)}{m}} \left(3 \pm \frac{1}{2} \left|\varphi_{\lambda}^{\mathtt{l}}\left(\frac{\omega_{1}}{M}\right)\right|\right).$$

Spectral analysis of any fixed initial positions and velocities

 $\psi(a,0) = \psi_0(a), \quad \dot{\psi}(a,0) = V_0(a),$

yields via the Hartley version of the forward honeycomb Fourier–Weyl C-transform (36) of type II from [7] the spectral functions $\hat{\psi}_0^{C,\pm}$, $\hat{V}_0^{C,\pm}$,

$$\widehat{\psi}_0^{C,\pm}(\lambda) = (12M^2 h_M(\lambda)\mu^{\pm}(\lambda))^{-1} \sum_{a \in H_M} \varepsilon(a)\psi_0(a)X_{\lambda}^{\pm}(a),$$
$$\widehat{V}_0^{C,\pm}(\lambda) = (12M^2 h_M(\lambda)\mu^{\pm}(\lambda))^{-1} \sum_{a \in H_M} \varepsilon(a)V_0(a)X_{\lambda}^{\pm}(a).$$

For the Neumann boundary conditions, the additional requirements $\widehat{\psi}_0^{C,-}([M,0,0]) = 0$ and $\widehat{V}_0^{C,-}([M,0,0]) = 0$ eliminate the translation mode and the resulting solution is of the form

$$\begin{split} \psi(a,t) &= \sum_{\lambda \in L_M} \left(\widehat{\psi}_0^{C,+}(\lambda) \cos(\omega_\lambda^+ t) + \frac{\widehat{V}_0^{C,+}(\lambda)}{\omega_\lambda^+} \sin(\omega_\lambda^+ t) \right) X_\lambda^+(a) \\ &+ \sum_{\lambda \in L_M \setminus [M,0,0]} \left(\widehat{\psi}_0^{C,-}(\lambda) \cos(\omega_\lambda^- t) + \frac{\widehat{V}_0^{C,-}(\lambda)}{\omega_\lambda^-} \sin(\omega_\lambda^- t) \right) X_\lambda^-(a). \end{split}$$

6 Conclusions

The discrete Fourier–Weyl transforms on finite fragments of the Weyl group invariant lattices are explicitly described in general forms in author's publications [7, 10, 12]. Boundary layouts of the point sets are for each root system dictated by the action of the sign homomorphisms on the generating reflections of the affine Weyl group. Besides the honeycomb lattice case, the point sets underlying in the discrete Fourier–Weyl transforms considered here are taken as finite subsets of the weight lattices. The root lattice discrete transforms [8] induce jointly with the weight lattice transforms fundamentally novel options for transforms on composed grids. The presented honeycomb lattice case, generated as subtraction of weight and root lattices of the root system A_2 [7], represents this approach for 2D lattices.

The completeness of the discretely orthogonal sets of the Weyl orbit functions in the finite-dimensional Hilbert spaces is guaranteed by coinciding cardinalities of the point and label sets [7, 10, 12]. A general algorithm for deriving the specific counting formulas for cardinalities of the point and label sets, which correspond to the dimensions of the functional Hilbert spaces, is developed in [10]. Further generalization of the algorithm for deriving counting formulas from [10] is applied for calculation of affine fusion tadpoles in conformal field theory [18]. The discretized versions of product-to-sum decomposition formulas lead to the dual weight lattice generalization of the Kac–Walton formula [11].

The properties of the unitary and symmetric Kac–Peterson matrices together with the affine fusion rules and Kac–Walton formulas [4] from conformal field theory motivated the development of the weight lattice discretization of Weyl orbit functions in [12]. The common argument and label symmetries of the weight lattice transforms, dictated by the affine Weyl groups, yield four types of unitary and symmetric generalizations of the Kac–Peterson matrices. The forms and physical significance of the generalized Kac–Walton formulas and Kac–Peterson matrices for all ten types of weight lattice discretized Weyl orbit functions need to be further investigated.

The Weyl orbit functions represent solutions of the mechanical vibration models constrained by Dirichlet, Neumann or mixed boundary conditions on the fundamental domain of the affine Weyl group. The discrete Fourier–Weyl and Hartley–Weyl transforms provide spectral analysis of given initial conditions and determine the explicit solutions. A significant advantage of the current symmetry approach for the honeycomb lattice [7] lies in the form of the resulting functions. Each solution is determined by a single Hartley honeycomb orbit function, whereas the standard approach yields two different functional descriptions, one for each congruence class of the honeycomb lattice [3, 14, 17]. Moreover, permitting an efficient interpolation [7], the honeycomb Fourier–Weyl and Hartley–Weyl C- and S-transforms thus represent suitable generalizations of the standard discrete cosine and sine transforms to the honeycomb lattice.

References

- N. Bourbaki, Groupes et algèbres de Lie, Chapiters IV, V, VI, Hermann, Paris (1968).
- [2] R. N. Bracewell, Discrete Hartley transform, J. Opt. Soc. Am. 73 (1983) 1832–1835.
- [3] J. Cserti, G. Tichy, A simple model for the vibrational modes in honeycomb lattices, Eur. J. Phys. 25 (2004) 723-736.
- [4] P. Di Francesco, P. Mathieu and D. Sénéchal, *Conformal field theory*, Springer, Berlin (1997).
- [5] L. B. Drissi, E. H. Saidi, M. Bousmina, Graphene, Lattice Field Theory and Symmetries, J. Math. Phys. 52 (2011) 022306.
- [6] J. Hrivnák, M. Juránek, On E-Discretization of Tori of Compact Simple Lie Groups. II, J. Math. Phys. 58 (2017) 103504.
- [7] J. Hrivnák, L. Motlochová, Discrete cosine and sine transforms generalized to honeycomb lattice, J. Math. Phys. 59 (2018) 063503.
- [8] J. Hrivnák, L. Motlochová, Dual root-lattice discretization of Weyl-orbit functions, J. Fourier Anal. Appl. 25 (2019) 2521–2569.
- [9] J. Hrivnák, L. Motlochová, J. Patera, On discretization of tori of compact simple Lie groups II, J. Phys. A: Math. Theor. 45 (2012) 255201.
- [10] J. Hrivnák, J. Patera, On discretization of tori of compact simple Lie groups, J. Phys. A: Math. Theor. 42 (2009) 385208.
- [11] J. Hrivnák, M. A. Walton, Discretized Weyl-orbit functions: modified multiplication and Galois symmetry, J. Phys. A: Math. Theor. 48 (2015) 175205.
- [12] J. Hrivnák, M. A. Walton, Weight-lattice discretization of Weyl-orbit functions, J. Math. Phys. 57 (2016) 083512.
- [13] R. Kane, Reflection Groups and Invariant Theory, New York, Springer, (2001).
- [14] T. Kariyado, Y. Hatsugai, Manipulation of Dirac Cones in Mechanical Graphene, Sci. Rep. 5 (2015) 18107.
- [15] A. Klimyk, J. Patera, Orbit functions, SIGMA 2 (2006) 006.
- [16] R. V. Moody, J. Patera, Orthogonality within the families of C-, S-, and E-functions of any compact semisimple Lie group, SIGMA 2 (2006) 076.
- [17] A. V. Rozhkov, F. Nori, Exact wave functions for an electron on a graphene triangular quantum dot, Phys. Rev. B 81 (2010) 155401.
- [18] A. Urichuk, M. A. Walton, Adjoint affine fusion and tadpoles, J. Math. Phys. 57 (2016) 061702.
- [19] M. A. Walton, On Affine Fusion and the Phase Model, SIGMA 8 (2012) 086.

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- J. Hrivnák, L. Motlochová, Discrete transforms and orthogonal polynomials of (anti)symmetric multivariate cosine functions, SIAM J. Numer. Anal. **52** (2014) 3021–3055.
- T. Czyżycki, J. Hrivnák, Generalized discrete orbit function transforms of affine Weyl groups, J. Math. Phys. 55 (2014) 113508.
- J. Hrivnák, J. Patera, On discretization of tori of compact simple Lie groups, J. Phys. A: Math. Theor. 42 (2009) 385208.
- P. Novotný, J. Hrivnák, On (α, β, γ)-derivations of Lie algebras and corresponding invariant functions, J. Geom. & Phys. 58 (2008) 208-217.