Decomposition of Plane Waves into Irreducible Representations of Space Groups

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Using a relation between representation theory of crystallographic space groups and a Dirichlet type of boundary problem for the Laplacian, we derive the solutions for the Dirichlet problem, as well as for a similar Neumann boundary problem, by a complete decomposition of plane waves into irreducible representations of a particular space group. This decomposition corresponds to a basis transformation in $L^2(\Omega)$ and yields a new set of basis functions adapted to the symmetry of the lattice considered.

Key words: Group Theory, Representation Theory, Boundary-Value problem, Basis Set for Band Calculations, Free Particle in a Box

1. Introduction

In a paper on the relation between semi-simple Lie algebras and crystallographic groups, Itzykson [1] investigates the spectrum of the Laplace operator on a fundamental domain of a space group of the A_n root lattice. This fundamental domain is bounded by a set of planes that generate this space group of the lattice by reflection. Thereby, a discussion on some particular eigenfunctions of the Laplace operator is performed. Those eigenfunctions vanish on the boundary of the fundamental domain. In papers by Berard [2] and Raszillier [3], one can find besides the Dirichlet type of problem also the corresponding Neumann boundary-value problem. However, in all cases an explicit construction of the eigenfunctions was omitted. The equivalent problem of a free quantum mechanical particle enclosed in a box was treated by Krishnamurthi, Mani, and Verma [4], and also by Turner [5].

In contrast to the papers cited above, we obtain the solutions for the Dirichlet as well as for the Neumann boundary condition via a basis transformation in the Hilbert space $L^2(\Omega)$, with Ω being a fundamental domain of a translation sublattice of the A_n root translation lattice. We decompose the plane waves as the starting basis set into irreducible spaces of representations. The advantage of such a decomposition

is evident from Schur's lemma, since an eigenvalue problem of a Hamiltonian that is invariant under transformation of the space group has to be solved only on the irreducible spaces of representations.

This concept is valid for various types of lattices, and the calculations presented for the A_2 root lattice should be understood as an example.

In Sect. 2 we formulate the boundary-value problem and show the relation to representation theory by extending the solution over the entire lattice. Furthermore, we consider the importance of the decomposition into irreducible spaces of representations. The explicit construction of those spaces is performed in section three in two steps. In step one we gain the representations of the space group via subduction from the representations of the translation group. Then we obtain the spaces by applying the Young operators to representations of the so-called little group. In Sect. 4 we close with a calculation in two dimensions.

2. Boundary-value problem and representation theory

The solutions of the free stationary Schrödinger equation (i.e. vanishing potential) are given by linear combinations of plane waves. In the following we denote by $\Omega \subset \mathbb{R}^n$ a fundamental domain (i.e. a set of points that generates the entire lattice under the group action) of a translation sublattice Λ of the A_n root translation lattice Γ. Then Ω has a finite

volume, and $\int_\Omega e^{-i\boldsymbol{K}\cdot\boldsymbol{x}}\mathrm{d}x$ vanishes for $0 \neq \boldsymbol{K} \in \Lambda_R = \{\boldsymbol{k}|\boldsymbol{k}\cdot\boldsymbol{a} \in 2\pi\mathbb{Z}, \boldsymbol{a} \in \Lambda\}$. Thus, the plane waves $e^{-i\boldsymbol{K}\cdot\boldsymbol{x}}$ ($\boldsymbol{K} \in \Lambda_R$) provide a basis of the Hilbert space $L^2(\Omega)$ on the one side and form a set of basis functions of the irreducible representation of the translation group on the other side. To preserve the translation group as a symmetry group, we can adopt periodic boundary conditions for the plane waves in $L^2(\Omega)$ (for instance Born- von Karman boundary conditions [6]).

On a polyhedron F bordered by $n+1$ affine hyperplanes, we are interested in finding solutions to the boundary-value problem

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\Delta\psi(\boldsymbol{x}) &= E\psi(\boldsymbol{x}) \quad \text{for} \quad \boldsymbol{x} \in F, \\
\psi(\boldsymbol{x}) &= 0 \qquad \text{for} \quad \boldsymbol{x} \in \partial F.
\end{aligned}
\tag{2.1}
$$

The space group $\mathcal{G}$ under consideration is the group, denoted by P_{n+1} in [7, p. 60]. It is generated by the reflections on these hyperplanes and has F as a fundamental domain. Formally, this space group is the semidirect product of the translation group and a particular point group of the lattice.

$$
\mathcal{G} = \boldsymbol{T} \otimes_{\boldsymbol{s}} \boldsymbol{W}.
\tag{2.2}
$$

At this point it shall be mentioned that we are not considering the holohedry of the lattice and that the point group $\boldsymbol{W}$ we are treating is isomorphic to the symmetric group S_{n+1} [8] and usually is called the Weyl group of the root lattice A_n. The fundamental domain F can be brought into the form [1]

$$
\begin{aligned}
F = \{\boldsymbol{x} \in \boldsymbol{V}\,|\,(\boldsymbol{x}\cdot\boldsymbol{f}_i) \geq 0, i = 1, \ldots, n, \\
\text{and } (-\boldsymbol{f}_0\cdot\boldsymbol{x}) \leq 1\}, \\
\text{where} \\
\boldsymbol{f}_0 = -\sum_{i=1}^n \boldsymbol{f}_i = -\sum_{i=1}^n (\boldsymbol{e}_i - \boldsymbol{e}_{i+1}) = \boldsymbol{e}_{n+1} - \boldsymbol{e}_1.
\end{aligned}
\tag{2.3}
$$

Here the $\boldsymbol{f}_i$, $i \neq 0$, denote the fundamental roots of the root lattice A_n, and $\boldsymbol{e}_i$ the standard Euclidean basis. One advantage of using the A_n lattices is that their fundamental roots generate the translation group as well as the point group.

As the plane waves ϕ_K satisfy the Schrödinger equation with $E = (\hbar|\boldsymbol{K}|)^2/2m$, it suffices to solve the boundary condition. In order to extend the solutions, which were at first confined to the fundamental domain of the space group to the entire lattice, we

use the irreducible representation $D_{k_0}^{\alpha_2}$ of $\mathcal{G}$ given by $D_{k_0}^{\alpha_2}(t, g) = \det(g)$ ($t \in \boldsymbol{T}, g \in \boldsymbol{W}$) and define

$$
\begin{aligned}
\psi(\boldsymbol{y}) &= \det(g)\psi(\boldsymbol{x}), \\
\text{if } \boldsymbol{y} &= c^{-1}\boldsymbol{x}, c = (t, g) \in \mathcal{G}, \boldsymbol{x} \in F;
\end{aligned}
\tag{2.4}
$$

observe $cF \cap F \subseteq \partial F$ for $c \neq e$. If U denotes the unitary representation of $\mathcal{G}$ on $L^2(\Omega)$ given by

$$
(U(c)\phi)(\boldsymbol{x}) = \phi(c^{-1}\boldsymbol{x}),
\tag{2.5}
$$

then the solution space of (2.1) is the $\mathcal{G}$-invariant subspace

$$
\{\phi \in L^2(\Omega)|U(c)\phi = D_{k_0}^{\alpha_2}(c)\phi, c \in \mathcal{G}\},
\tag{2.6}
$$

sometimes called the homogeneous component with respect to the given irreducible representation of $\mathcal{G}$, observe $D_{k_0}^{\alpha_2}(c) = -1$ for reflections c in $\mathcal{G}$. This connection motivates us to study in a more general scope the decomposition of $L^2(\Omega)$ into homogeneous components and to determine a basis which corresponds to this decomposition.

3. Induced representations and Young operators

The method of inducing a representation enables us to construct the irreducible spaces of representations for a space group by knowing the irreducible representations of the translation group and the specific point group.

First of all, we calculate the so-called little group. For this purpose we decompose the space group into cosets.

$$
\mathcal{G} = a_1\boldsymbol{T} + \ldots + a_n\boldsymbol{T}.
\tag{3.7}
$$

Since $\boldsymbol{T}$ is an invariant subgroup of $\mathcal{G}$, we have besides the irreducible representations

$$
D^k(t) = e^{i(\boldsymbol{k}\cdot\boldsymbol{t})}
\tag{3.8}
$$

also representations of the form

$$
D_i^k = \{D_i^k(t)\,|\,t \in \boldsymbol{T}\}, \; D_i^k(t) = D^k(a_i^{-1}ta_i).
\tag{3.9}
$$

Here $\boldsymbol{k}$ is a point of the first Brillouin zone (BZ). The BZ is a fundamental domain with respect to the group of the reciprocal lattice translation. Therefore any vector $\boldsymbol{K}$ admits a decomposition $\boldsymbol{K} = \boldsymbol{K}_R + \boldsymbol{k}$ with $\boldsymbol{K}_R \in \Gamma^R$. For fixed $\boldsymbol{k}$ we denote those a_i that

lead to equivalent representations of the translation group as $r_i^{(k)}$. These $r_i^{(k)}$ define the little group in the following way:

$$L_k^{II} = r_1^{(k)} T + \dots + r_s^{(k)} T. \qquad (3.10)$$

If we make use of a notation which suits the semidirect structure of the space group and write the $r_i^{(k)}$ as $(0, g_i)$ [1], where $g_i \in W$, and t becomes (t, e), then from (3.8) we obtain

$$
\begin{aligned}
D^k((0, g_i^{-1})(t, e)(0, g_i)) &= D^k(g_i^{-1} t, e) \\
&= D^{g_i k}(t, e),
\end{aligned}
\qquad (3.11)
$$

where we used $(g_i^{-1}) = (g_i)^T$, and the condition for the little group reads

$$L_k^{II} = T \otimes_s L_k^I, L_k^I = \{h \in W | D^{hk} = D^k\}. \quad (3.12)$$

Usually [9], [10] L_k^{II} and L_k^I are called little group of the second kind and little group of the first kind, respectively. We will call them little groups and carry the indices for distinction.

Apparently, the little group depends on k. To classify all possible little groups, we have to analyze the first Brillouin Zone of the reciprocal lattice of the root lattice. The irreducible representations of the little group are easily seen to be of the form

$$D^{k, \alpha_i} = D^k \otimes D^{\alpha_i}. \qquad (3.13)$$

Here the D^{α_i} stand for the irreducible representations of L_k^I. If we now decompose the space group into cosets with respect to the little group

$$\mathcal{G} = (0, c_1) L_k^{II} + \dots + (0, c_m) L_k^{II}, \qquad (3.14)$$

we get irreducible representations, more accurately the matrix elements of the space group as induced representations of the form

$$D_{ij}^{k, \alpha}(t, g) = \delta(c_i^{-1} g c_j, h) D^{c_i k, \alpha}(t, h),$$

$$\text{where } \delta(c_i^{-1} g c_j, h) = \begin{cases} 1 : c_i^{-1} g c_j = h \in W, \\ 0 : \text{otherwise.} \end{cases}$$

However, we are interested in functions that transform like the irreducible representations of the space group. The method of inducing representations does also provide those functions [10], as long as a basis is

known for the subgroup we induce from. If this basis is given as $\{\phi_K^\alpha\}$, the associated basis for the induced representation is given by

$$\phi_K^{\alpha, i}(x) := \phi_K^\alpha(c_i^{-1} x), \ K = K_R + k. \qquad (3.15)$$

Thus, the remaining task is to construct the irreducible subspaces of representations of the little group. For this purpose we apply the so-called Young operators [11] to the plane waves, which transform like the irreducible representations of the translation group. If we consider, for a fixed $k \in BZ$, an irreducible representation D^α of L_k^I of dimension d^α, then the associated Young operator is

$$P_{ij}^\alpha = \frac{d^\alpha}{|L_k^I|} \sum_{h \in L_k^I} D_{ij}^\alpha(h)^* U(0, h). \qquad (3.16)$$

By a straightforward calculation, we can see that the functions $\psi_i(x) = [P_{ij}^\alpha \phi_K](x)$, with $\phi_K(x) = e^{-i(K \cdot x)}$, in fact satisfy for every j the desired transformation property. Using (2.5) and (3.12) we find

$$
\begin{aligned}
&U(t_0, h_0)(P_{ij}^\alpha \phi_K)(x) \\
&= \frac{d^\alpha}{|L_k^I|} \sum_{h \in L_k^I} D_{ij}^\alpha(h)^* [U(t_0, h_0) U(0, h) \phi_K](x) \\
&= \frac{d^\alpha}{|L_k^I|} \sum_{h \in L_k^I} D_{ij}^\alpha(h)^* [U(0, h_0 h) \\
&\qquad\qquad \times [U((h_0 h)^{-1} t_0, e) \phi_K](x) \quad (3.17) \\
&= \frac{d^\alpha}{|L_k^I|} \sum_{h \in L_k^I} e^{i([h_0 h] k) \cdot t_0} D_{ij}^\alpha(h_0^{-1} h_0 h)^* \\
&\qquad\qquad \times [U(0, h_0 h) \phi_K](x) \\
&= e^{ik \cdot t_0} \sum_l D_{li}^\alpha(h_0)(P_{lj}^\alpha \phi_K)(x).
\end{aligned}
$$

Observe, that the $(d^\alpha)^2$ functions $[P_{ij}^\alpha \phi_K](x)$ may be linearly dependent. But, if all groups L_k^I and their irreducible representations are classified, we are able to construct the irreducible subspaces of representations of the space group in $L^2(\Omega)$.

4. The decomposition in two dimensions

The A_2 root lattice shall now illustrate the decomposition in two dimensions explicitly. The translation

group and the Weyl group are then given by

$$T = \{t \mid t = n_1 f_1 + n_2 f_2\},$$
$$f_1 = e_2 - e_1, \; f_2 = e_3 - e_2$$
$$W = < S_1, S_2 \mid S_i^2 = (S_1 S_2)^3 = e >$$
$$= \{e, S_1, S_2, S_3, d_1, d_2\}$$

(4.18)

with the generating relations

$$S_1 S_2 = d_1,$$
$$S_2 S_1 = d_2,$$
$$S_1 S_2 S_1 = S_2 S_1 S_2 = S_3.$$

(4.19)

The Dirichlet problem in two dimensions becomes

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right)\psi(x) = E\psi(x), \quad x \in F,$$
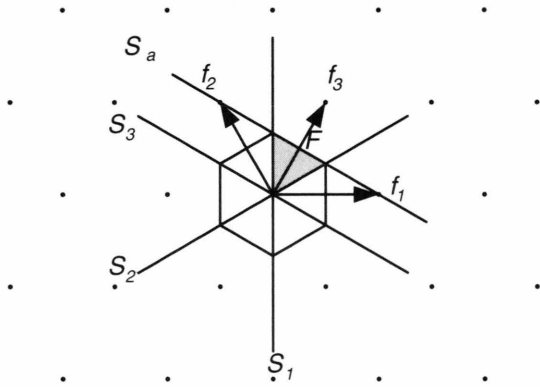$$\psi(x) = 0, \qquad x \in \partial F.$$

(4.20)

Fig. 4.1. Fundamental domain within the Wigner-Seitz cell of the A_2.

In Fig. 4.1, the fundamental reflections S_1 and S_2 are represented by lines. These reflections, together with one affine reflection S_a, generate on the one side the space group under consideration and on the other side a space filling tiling of $\mathbb{R}^2$ via the fundamental domain F.

The first step in our procedure is to classify all possible little groups. The defining condition was given in (3.12), which also can be stated in the form

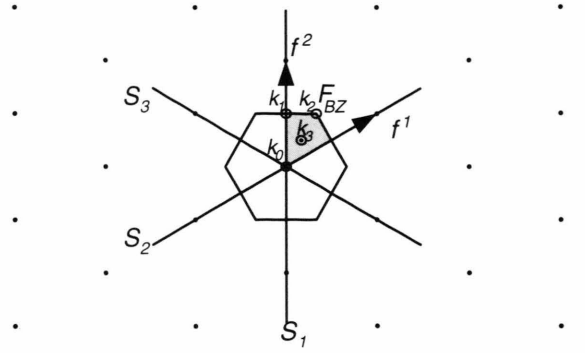$$L_k^{II} = T \otimes_S L_k^I, \; L_k^I = \{h \in W \mid hk - k \in \Gamma^R\}.(4.21)$$

Fig. 4.2. Fundamental domain of the first Brillouin Zone.

Apparently (Fig. 4.2), many $k \in BZ$ lead to isomorphic little groups, and it is sufficient to consider only a certain number of representative $k \in BZ$. Furthermore, it can be proved that $L_{qk}^I = qL_k^I q^{-1}$. Thus, we can concentrate our analysis to $k \in F_{BZ}$, the sector of BZ which is part of the fundamental domain for the point group. The dots that are marked with k_i, $i = 0, .., 3$, stand for the four possible classes and hence four different little groups. These k indicate different irreducible representations of the space group, and in three dimensions, in contrast to two dimensions, a standard notation with capital Roman ($k \in \partial BZ$) and Greek ($k \in BZ$) letters [10] is used. The four little groups are given by

$$L_{k_0}^I = \{e, S_1, S_2, S_3, d_1, d_2\},$$
$$L_{k_1}^I = \{e, S_1\},$$
$$L_{k_2}^I = \{e, d_1, d_2\},$$
$$L_{k_3}^I = \{e\}.$$

(4.22)

For $L_{k_0}^I$ we have three different irreducible representations, which we denote by D^{α_i}:

$$D_{k_0}^{\alpha_1} : \{D^{\alpha_1}(h) = 1 \mid \forall h \in L_{k_0}^I\},$$

(4.23)

$$D_{k_0}^{\alpha_2} : \{D^{\alpha_2}(e) = D^{\alpha_2}(d_1) = D^{\alpha_2}(d_2) = 1;$$
$$D^{\alpha_2}(S_i) = -1, \; i = 1, 2, 3\},$$

$$D_{k_0}^{\alpha_3} : \begin{cases} D^{\alpha_3}(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ D^{\alpha_3}(d_1) = \begin{pmatrix} e^{-i\frac{2}{3}\pi} & 0 \\ 0 & e^{i\frac{2}{3}\pi} \end{pmatrix} \\ D^{\alpha_3}(d_2) = \begin{pmatrix} e^{i\frac{2}{3}\pi} & 0 \\ 0 & e^{-i\frac{2}{3}\pi} \end{pmatrix} \\ D^{\alpha_3}(S_1) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ D^{\alpha_3}(S_2) = \begin{pmatrix} 0 & e^{i\frac{2}{3}\pi} \\ e^{-i\frac{2}{3}\pi} & 0 \end{pmatrix} \\ D^{\alpha_3}(S_3) = \begin{pmatrix} 0 & e^{-i\frac{2}{3}\pi} \\ e^{i\frac{2}{3}\pi} & 0 \end{pmatrix} \end{cases}.$$

$L_{k_1}^I$ only yields two irreducible representations:

$$D_{k_1}^{\beta_1} : \{D^{\beta_1}(e) = 1 \mid D^{\beta_1}(S_1) = 1\},$$
$$D_{k_1}^{\beta_2} : \{D^{\beta_2}(e) = 1 \mid D^{\beta_2}(S_1) = -1\}. \quad (4.24)$$

Finally, we obtain three irreducible representations for $L_{k_2}^I$

$$D_{k_2}^{\gamma_1} : \{D^{\gamma_1}(e) = D^{\gamma_1}(d_1) = D^{\gamma_1}(d_1) = 1\},$$
$$D_{k_2}^{\gamma_2} : \{D^{\gamma_2}(e) = 1, \ D^{\gamma_2}(d_1) = e^{i\frac{2}{3}\pi},$$
$$D^{\gamma_2}(d_2) = e^{-i\frac{2}{3}\pi}\}, \quad (4.25)$$
$$D_{k_2}^{\gamma_3} : \{D^{\gamma_3}(e) = 1, \ D^{\gamma_3}(d_1) = e^{-i\frac{2}{3}\pi},$$
$$D^{\gamma_3}(d_2) = e^{i\frac{2}{3}\pi}\},$$

and one irreducible representation for the trivial case of $L_{k_3}^I$:

$$D_{k_3}^{\delta}(e) = 1. \quad (4.26)$$

Those irreducible representations define the various Young operators, and by applying these operators to the plane waves we find the functions that have the proper transformation property. In order to obtain a new basis for $L^2(\Omega)$, we have to make sure that all plane waves, i.e. every $K_R \in \Gamma_R$ (reciprocal lattice), appear in the decomposition. For this purpose it is useful to consider the orbit of K_R, i.e. gK_R for all $g \in W$. Generally, we find orbits of order six and orbits of order three (K_R lying in a reflection plane). Thus, the decomposition is complete if for a given little group and given orbit those six or three linear combinations are determined that have the correct

transformation property.
Again we start with the representations of $L_{k_0}^I$:

$$[P^{\alpha_1}\phi_{K_R}](x) = \tfrac{1}{6}[e^{-iK_R\cdot x} + e^{-i(d_1 K_R)\cdot x}$$
$$+ e^{-i(d_2 K_R)\cdot x} + e^{-i(S_1 K_R)\cdot x}$$
$$+ e^{-i(S_2 K_R)\cdot x} + e^{-i(S_3 K_R)\cdot x}],$$
$$[P^{\alpha_2}\phi_{K_R}](x) = \tfrac{1}{6}[e^{-iK_R\cdot x} + e^{-i(d_1 K_R)\cdot x} \quad (4.27)$$
$$+ e^{-i(d_2 K_R)\cdot x} - e^{-i(S_1 K_R)\cdot x}$$
$$- e^{-i(S_2 K_R)\cdot x} - e^{-i(S_3 K_R)\cdot x}].$$

For the two dimensional representation we obtain

$$\begin{cases} [P_{11}^{\alpha_3}\phi_{K_R}](x) = \tfrac{1}{3}[e^{-iK_R\cdot x} + e^{i\frac{2}{3}\pi}e^{-i(d_1 K_R)\cdot x} \\ \qquad + e^{-i\frac{2}{3}\pi}e^{-i(d_2 K_R)\cdot x}], \\ [P_{21}^{\alpha_3}\phi_{K_R}](x) = \tfrac{1}{3}[e^{-i(S_1 K_R)\cdot x} + e^{i\frac{2}{3}\pi}e^{-i(S_2 K_R)\cdot x} \\ \qquad + e^{-i\frac{2}{3}\pi}e^{-i(S_3 K_R)\cdot x}], \end{cases} \quad (4.28)$$

$$\begin{cases} [P_{12}^{\alpha_3}\phi_{K_R}](x) = \tfrac{1}{3}[e^{-iS_1 K_R\cdot x} + e^{-i\frac{2}{3}\pi}e^{-i(S_2 K_R)\cdot x} \\ \qquad + e^{i\frac{2}{3}\pi}e^{-i(S_3 K_R)\cdot x}], \\ [P_{22}^{\alpha_3}\phi_{K_R}](x) = \tfrac{1}{3}[e^{-iK_R\cdot x} + e^{-i\frac{2}{3}\pi}e^{-i(d_1 K_R)\cdot x} \\ \qquad + e^{i\frac{2}{3}\pi}e^{-i(d_2 K_R)\cdot x}]. \end{cases} \quad (4.29)$$

The parentheses are used to distinguish between the two different subspaces of the same irreducible representations for fixed reciprocal lattice vector K_R.

In the case, where $L_{k_0}^{II}$ is identical with the space group, we already have the complete set of new basis functions.

For $L_{k_1}^I$ we derive the two functions

$$[P^{\beta_1}\phi_{K_R+k_1}](x) = \frac{1}{2}[e^{-i[K_R+k_1]\cdot x} + e^{-i(S_1[K_R+k_1])\cdot x}],$$
$$[P^{\beta_2}\phi_{K_R+k_1}](x) = \frac{1}{2}[e^{-i[K_R+k_1]\cdot x} - e^{-i(S_1[K_R+k_1])\cdot x}]. \quad (4.30)$$

Here we only have two functions. According to (3.15) we can complete the irreducible subspace by taking $[P^{\beta_i}\phi_{K_R+k_1}](c_j^{-1}x)$, with $c_j = e, d_1, d_2$, respectively, which are the coset generators for $L_{k_1}^I$ with respect to W. This is equivalent to taking two other plane waves belonging to the same orbit and repeating the

projection formalism.

Similary, we obtain for $L_{k_2}^I$:

$$[P^{\gamma_1}\phi_{K_R+k_2}](\boldsymbol{x}) = \tfrac{1}{3}[e^{-i[K_R+k_2]\cdot\boldsymbol{x}} + e^{-i(d_1[K_R+k_2])\cdot\boldsymbol{x}}$$
$$+ e^{-i(d_2[K_R+k_2])\cdot\boldsymbol{x}}],$$

$$[P^{\gamma_2}\phi_{K_R+k_2}](\boldsymbol{x}) = \tfrac{1}{3}[e^{-i[K_R+k_2]\cdot\boldsymbol{x}}$$
$$+ e^{-i\frac{2}{3}\pi}e^{-i(d_1[K_R+k_2])\cdot\boldsymbol{x}}$$
$$+ e^{i\frac{2}{3}\pi}e^{-i(d_2[K_R+k_2])\cdot\boldsymbol{x}}],$$ (4.31)

$$[P^{\gamma_3}\phi_{K_R+k_2}](\boldsymbol{x}) = \tfrac{1}{3}[e^{-i[K_R+k_2]\cdot\boldsymbol{x}}$$
$$+ e^{i\frac{2}{3}\pi}e^{-i(d_1[K_R+k_2])\cdot\boldsymbol{x}}$$
$$+ e^{-i\frac{2}{3}\pi}e^{-i(d_2[K_R+k_2])\cdot\boldsymbol{x}}],$$

where this set is completed by $[P^{\gamma_i}\phi_{K_R+k_2}](c_j^{-1}\boldsymbol{x})$, with $c_j = e, S_1$ denoting the coset generators for $L_{k_2}^I$. Finally, we have

$$[P^\delta\phi_{K_R+k_3}](g^{-1}\boldsymbol{x}) = e^{-i(g[K_R+k_3])\cdot\boldsymbol{x}}, \ \forall g \in W \ (4.32)$$

as the last class of subspaces for this particular space group decomposition.

Actually, a procedure to obtain the complete set of new basis functions in a rather direct way can be stated as follows: For a given little group $L_{k_i}^I$ apply the associated Young operators to all plane waves belonging to an orbit and choose a maximum set of linear independent functions. One way to achieve this set of linear independent functions right away is to confine the reciprocal lattice vectors of this orbit to certain Weyl chambers (fundamental regions [12]). In the case of A_2 the reciprocal lattice can be divided into six regions that all represent a fundamental region with respect to the Weyl group. Now for every little group $L_{k_i}^I$ the K_R will be taken only from a certain number of Weyl chambers that is given by $|W|/|L_{k_i}^I|$. Still we have the freedom which chambers we choose as long as they are adjacent to each other.

4.1 Dirichlet and Neumann boundary-value problem in two dimensions

The problem we started with was to find solutions to a Dirichlet boundary-value problem by determining a basis of the space (2.6), which belongs to the symmetry adapted basis of $L^2(\Omega)$. Although we started with the Dirichlet problem, we find that the other

one-dimensional representation $D_{k_0}^{\alpha_1}$ solves a similar problem for Neumann boundary conditions. For this purpose we write the one-dimensional representations in a slightly different form (in the following $\det(g)$ denotes the determinant of the representation $D_{k_0}^{\alpha_3}$ (4.23)):

$$\psi^D(\boldsymbol{x}) = 6[P^{\alpha_2}\phi_{K_R}](\boldsymbol{x}) = \sum_{g\in W} \det(g)e^{-i(gK_R)\cdot\boldsymbol{x}}.$$
$$\psi^N(\boldsymbol{x}) = 6[P^{\alpha_1}\phi_{K_R}](\boldsymbol{x}) = \sum_{g\in W} e^{-i(gK_R)\cdot\boldsymbol{x}}.$$

For the Dirichlet type of problem we now know that the functions $\psi^D(\boldsymbol{x})$, $K_R \neq 0$, provide a basis for the solution space.

For Neumann boundary condition we have to prove for any $\boldsymbol{x} \in \partial F$:

$$\frac{\partial\psi^N}{\partial\boldsymbol{n}}(\boldsymbol{x}) = (\boldsymbol{n} \cdot \nabla\psi^N(\boldsymbol{x})) = 0.$$

Hereby the normal vector $\boldsymbol{n}$ is given by one of the three vectors $\boldsymbol{f}_j$ ($j = 0, 1, 2$), $\boldsymbol{f}_0 = -\boldsymbol{f}_3$, cf. (2.3). Further, with $S_0 = S_a$, we have $S_j\boldsymbol{f}_j = -\boldsymbol{f}_j$. For $\boldsymbol{x}$ lying on the reflection planes the condition $S_j\boldsymbol{x} = \boldsymbol{x}$ results in

$$(\boldsymbol{f}_j \cdot \nabla\psi^N(S_j\boldsymbol{x})) = (\boldsymbol{f}_j \cdot \nabla\psi^N(\boldsymbol{x})).$$

On the other hand, an explicit calculation yields $\nabla\phi_{K_R}(x) = -iK_R\phi_{K_R}(x)$ and

$$(\boldsymbol{f}_j \cdot \nabla\psi^N(S_j\boldsymbol{x}))$$
$$= -i\sum_{g\in W}(\boldsymbol{f}_j \cdot S_jgK_R)e^{-i(S_jgK_R)\cdot\boldsymbol{x}}$$
$$= -i\sum_{g\in W}(S_j\boldsymbol{f}_j \cdot gK_R)e^{-i(gK_R)\cdot\boldsymbol{x}}(\boldsymbol{f}_j \cdot \nabla\psi^N(S_j\boldsymbol{x}))$$
$$= i\sum_{g\in W}(\boldsymbol{f}_j \cdot gK_R)e^{-i(gK_R)\cdot\boldsymbol{x}}$$
$$= -(\boldsymbol{f}_j \cdot \nabla\psi^N(\boldsymbol{x})),$$

and our proof is complete.

5. Concluding remarks

The main task of this paper is to decompose the plane waves into subspaces of irreducible representations for a given space group of A_n. The two reasons we were guided by were to provide a symmetry adapted basis set for band structure calculations in a

crystal and to find the solutions to a Dirichlet type of boundary-value problem. The A_n root lattice is used because of its simple relation between primitive vectors and normal vectors of bounding planes of the fundamental domain. Nevertheless, similar calculations can be performed on various types of crystallographic symmetry structures. Since the boundary-value problem has been discussed extensively, we will only comment on the first point. The computation of band structures always requires some approximations. One of the standard methods [6] is the so-called muffin-tin approximation, where the primitive cell is divided into a region with constant potential (interstitial region) and a region with spherical potential about the lattice site. The APW-method (augemented plane waves) takes plane waves to approximate the solutions in the interstitial region. Since a spherical potential commutes with any point group operation, it is sufficient with the present method to perform the calculations on the decomposed subspaces for fixed $k \in BZ$. Thus, the numerical effort is reduced in the case of A_2 up to a factor of $(2 + 1)! = 6$. For A_n we find a maximum factor of $(n + 1)!$ which helps to simplify the calculations a great deal.

Acknowledgements

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