Symmetry properties of the density of states in the Brillouin zone for a one-dimensional periodic Heisenberg magnet

Symmetry properties of the density of states in the Brillouin zone for a one-dimensional periodic Heisenberg magnet

W Florek and T Lulek

Institute of Physics, A Mickiewicz University, Poznań, Poland

Abstract. Symmetry properties of the density of states in the Brillouin zone for the Heisenberg model of a finite one-dimensional magnetic crystal are investigated using a general prescription of Weyl, which consists here in an analysis of the action of the ring of endomorphisms of a cyclic group in the space of quantum states of the magnet. It is shown that the density of states is constant on orbits of the group of automorphism in the Brillouin zone. Each such orbit can be thus interpreted as a generalised star of a wavenumber. It is also shown that the distribution of states in the discrete one-dimensional Brillouin zone is governed by some selection rules on the lattice (i.e. partially ordered set with unique maximal and minimal elements) of subgroups of the cyclic group.

1. Introduction

In this paper, which is an extension of a paper by one of us (Lulek 1984, hereafter referred to as I), we consider some symmetry aspects of the space of quantum states of a finite linear chain, consisting of N spins s, distributed in nodes of the chain according to the symmetry of the cyclic group C_N. Such a system provides a one-dimensional finite version of the model of a magnet with localised carriers of the magnetic moment ('spins'), introduced by Heisenberg (1928, see also Mattis 1965, §§ 2 and 7, and Dyson 1956, and references therein) to explain the origin of magnetism in crystal insulators. The space of quantum states of the Heisenberg model of a magnet constitutes the tensor product of N copies of $(2s+1)$-dimensional single-node spaces spanned on standard $|sm\rangle$ states of the spin s. A similar construction of the space of quantum states is intrinsic in the Ising model (Ising 1925, see also Newell and Montroll 1953). Due to such a construction of the space of quantum states, the Heisenberg, Ising and some related models proved to be useful tools, not only for a description of magnetic properties of crystals, but also found thorough applications in several other problems of quantum statistical physics, such as phase transitions (Wilson and Kogut 1974, Bak 1982), coherence (Dicke 1954, Takahashi and Shibata 1975), disordered crystals (Elliott *et al* 1974), defects in crystals (Mermin 1979) and others. A particularly important role is associated with the one-dimensional magnet with periodic boundary conditions considered in the present paper, since the relative simplicity of the spatial distribution of nodes in the linear chain yields mathematically rigorous results for this case, and, on the other hand, the actual state of technology allows us to investigate experimentally several magnetic systems which are well described by such a model (see Bonner 1978 and references therein). Such linear models are also

applied in theoretical searching for superconductivity in organic crystals (Allender *et al* 1974 and references therein), or in attempts for modelling some biological processes (Tsetlin 1969, Reiss 1964).

The problem considered here is associated with the distribution of quantum states of the magnet over the one-dimensional Brillouin zone, defined as the set of wavenumbers k, i.e. of exact quantum numbers resulting from the translational symmetry of the model. To state our problem precisely, we propose the following notation. Let

$$\tilde{N} = \{j \,|\, j = 1, 2, \ldots, N\} \tag{1}$$

be the set of integers, $1, \ldots, N$,

$$C_N = \{\tilde{N}, \text{`+'} \bmod N\} \tag{2}$$

be the cyclic group in additive notation,

$$\sigma = \begin{pmatrix} j \\ \sigma(j) \end{pmatrix} = \begin{pmatrix} \bar{\sigma}(j) \\ j \end{pmatrix} \qquad j \in \tilde{N} \tag{3}$$

be a permutation on the set $\tilde{N}$ (so that $\sigma(j)$ and $\bar{\sigma}(j)$ are the image and counterimage of the element $j \in \tilde{N}$ under the permutation σ respectively), and let $\Sigma_N = \{\sigma\}$ be the symmetric group on the set $\tilde{N}$. The formula

$$\sigma_j = \begin{pmatrix} j' \\ (j+j') \bmod N \end{pmatrix} \in \Sigma_N \qquad j \in C_N \qquad j' \in \tilde{N} \tag{4}$$

defines an embedding of the cyclic group C_N into the symmetric group Σ_N. The embedding $C_N \subset \Sigma_N$ defines in the set $\tilde{N}$ a cyclic order (Hall 1967), consistent modulo N with the natural order for the ring Z of integers. The set $\tilde{N}$ with this cyclic order will be identified with the set of nodes of a one-dimensional magnetic crystal subjected to periodic Born–Karman boundary conditions (with a magnetic linear chain) and the group C_N given by equation (2), with its action on $\tilde{N}$ given by equation (4), as the translation group of this crystal. The linear chain $\tilde{N}$ thus constitutes an orbit of the regular representation of the group C_N, and the cyclic order determines the sequence of nodes with respect to an (arbitrarily chosen) initial node.

The natural assumption of invariance of the Hamiltonian of the magnetic chain with respect to the group C_N of the symmetry of the geometric distribution of nodes implies that the irreducible representations Γ_k of this group over the field C of complex numbers, given by the characters

$$\chi^{\Gamma_k}(j) = \exp(2\pi i k j / N) \qquad j \in C_N \tag{5}$$

are exact quantum numbers for stationary states of the magnet. Therefore, the set

$$B = \left\{ k \,\middle|\, k = 0, \pm 1, \pm 2, \ldots, \begin{array}{ll} \pm(N/2-1), N/2 & \text{for } N \text{ even} \\ \pm(N-1)/2 & \text{for } N \text{ odd} \end{array} \right\} \tag{6}$$

of wavenumbers k admissible by periodic conditions constitutes a finite equivalent of the one-dimensional Brillouin zone $B' = (-\pi, \pi]$, i.e. the set of (classes of linear equivalence of) irreducible representations (over C) of the translation group of the crystal (we use here, for convenience of notation, integer k, which differ from standard spectroscopic wavenumbers by a factor $2\pi/a$, with a being the lattice constant of the crystal). We hereafter refer to B as the Brillouin zone of the crystal $\tilde{N}$. In particular, the wavenumber $k = 0$ corresponds to the centre of the Brillouin zone B, and for N even there exist $k = N/2$, the boundary of the zone B.

Let $m = -s, -s+1, \ldots, s$, be standard magnetic quantum numbers of the single-node spin s. For convenience of notation, we will denote these quantum numbers by the label $i \in \tilde{n} = \{1, \ldots, n\}$, $n = 2s+1$, by putting $m_i = -s - 1 + i$. Then the linear closure lc $\tilde{n}$ of formal linear combinations of elements of the set $\tilde{n}$ over the field C constitutes the space of quantum states of a single-node spin, and the linear space

$$L = \prod_{j \in \tilde{N}} \otimes (\text{lc } \tilde{n})_j \tag{7}$$

i.e. the tensor product of N copies $(\text{lc } \tilde{n})_j$, $j \in \tilde{N}$, of the single-node space lc $\tilde{n}$ is the space of quantum states of the whole magnet. Moreover, the set

$$\tilde{n}^{\tilde{N}} = \{f : \tilde{N} \to \tilde{n}\} \equiv \{|i_1, \ldots, i_N\rangle \mid i_j \in \tilde{n} \text{ for } j \in \tilde{N}\} \tag{8}$$

of all mappings of the set $\tilde{N}$ of nodes of the magnet into the set $\tilde{n}$ of single-node spin states (assumed to be orthonormal in lc $\tilde{n}$), constitutes an orthonormal natural basis in the unitary space L, so that

$$L = \text{lc } \tilde{n}^{\tilde{N}} \qquad \dim L = n^N = (2s+1)^N. \tag{9}$$

For example, the mapping $f \equiv |n, \ldots, n\rangle$, i.e. the mapping given by $f(j) = n, j \in \tilde{N}$, corresponds to a ground state of a ferromagnet, with all single-node spins aligned, which yields the maximal magnetisation directed along the quantisation axis.

The action of the group Σ_N on the set $\tilde{N}$ generates in a natural way the permutation representation P on the set $\tilde{n}^{\tilde{N}}$ by the formula

$$P(\sigma)|i_1, \ldots, i_N\rangle = |i_{\tilde{\sigma}(1)}, \ldots, i_{\tilde{\sigma}(N)}\rangle \qquad \sigma \in \Sigma_N \qquad |i_1, \ldots, i_N\rangle \in \tilde{n}^{\tilde{N}}. \tag{10}$$

By a natural extension, P becomes a linear representation acting in the space L. The decomposition of the subduction $P \downarrow C_N$ of the linear representation P to the subgroup $C_N \subset \Sigma_N$ into irreducible representations Γ_k, $k \in B$, of the translation group C_N, given by the formula

$$P \downarrow C_N \simeq \sum_{k \in B} \oplus \rho(k) \Gamma_k \tag{11}$$

where $\rho(k)$ is the multiplicity of Γ_k in P (i.e. the number of linearly independent states of the magnet with a given wavenumber k from the Brillouin zone B), determines the mapping $\rho : B \to Z$, referred (after I) to as the density of states in the Brillouin zone.

An analytic formula for the mapping ρ has been given in I. It follows that, in general, the density ρ is not homogeneous in the Brillouin zone B, contrary to the text-book case of the density of quantum states of a free particle inside a box or a one-dimensional potential well. In a sense, the mapping $\rho : B \to Z$ can be treated as a discrete analogue of the mapping $\rho' : B' \to R$ of the continuous Brillouin zone B' for the infinite linear chain into the field R of real numbers, so that $\rho'(k')$ is the density of states at $k' \in B'$. For example, for the one-dimensional motion of a spinless free particle in a potential well we have for the lowest band $\rho' = 1/2\pi$, so that this density is homogeneous in the whole Brillouin zone B'. The corresponding homogeneity for the three-dimensional motion of a free electron in a box provides, together with the Pauli exclusion principle, the ground for the notion of the Fermi surface. This homogeneous density ρ' is essentially a result of the first law of Newton, i.e. of the assumption of mechanical equivalence of all inertial reference frames, implicit in the notion of a free particle (despite the existence of the physically distinguished reference frame—that in which the box or well rests). We intend to investigate the nature of the inhomogeneity of the density ρ in the Brillouin zone B in this paper. In particular,

we are going to point out the regions of constant density and describe the symmetry of the distribution of inhomogeneities.

The solution of the above problem happens to be essentially a realisation of a general prescription given by Weyl (1952, see also Mozrzymas 1976, Lulek *et al* 1985a), according to which all invariant properties of a physical model can be drawn by means of detailed analysis of the groups of automorphisms of the mathematical structure used for a formal description of the model. This prescription can be looked at as an extended version of the postulate of relativity.

The mathematical tools used here to present a solution of the problem are dissipated over several branches like the theory of Abelian groups (Fuchs 1970, Hall 1959, Kurosh 1960, Mozrzymas 1976), theoretical arithmetics (Hasse 1979, Narkiewicz 1977) or the theory of lattices with the associated combinatorics (Hall 1967, Rybnikov 1972, Satschkov 1977, Grätzer 1978), and involve such notions as rings, lattices, endomorphisms, orbits, socles, etc. Essentially, the main body of the paper is organised with the intention of exposing only the most important aspects of the realisation of the Weyl prescription, whereas details like definitions and theorems from several branches of mathematics involved in the presentation of the solution, as well as a natural, 'physical' interpretation of some notions, are collected in two appendices (with some repetition ensuring continuity of presentation).

2. A realisation of Weyl's prescription

According to the prescription of Weyl, we have to study the group $\mathrm{Aut}\, C_N$ of all automorphisms of the group C_N for translations of the physical system with its action in the space L of quantum states. In our case it happens that a much more thorough description of the physical situation can be achieved by considering a little more general structure, namely the ring $\mathrm{End}\, C_N$ of all endomorphisms of the group C_N, enclosing $\mathrm{Aut}\, C_N$ as its multiplicative group.

A detailed description of the structure of the ring $\mathrm{End}\, C_N$, needed to define and analyse the action of an arbitrary endomorphism $\eta_1 \in \mathrm{End}\, C_N$, $l \in \tilde{N}$, in the space L of states of our magnet, is collected in appendices 1 and 2. Here, we only mention an important role of the arithmetic structure of the integer N, i.e. of the decomposition (A1.1) into prime factors p ('atoms' of N), since this leads in a natural way to the notion of the lattice $K(N)$ of subgroups of the group C_N. The elements of $K(N)$, i.e. the subgroups of C_N, are classified by divisors κ of N. We shall show that the invariant properties of the considered density of states are adequately described in terms of elements of the lattice $K(N)$ only. Appendix 1 contains a geometric presentation of the lattice $K(N)$ as a transmission circuit in a form of a finite simple hypercubic lattice, with the minimal ($\kappa = 1$) and maximal ($\kappa = N$) elements being the input and output respectively. The 'elementary cell' in this lattice is spanned by the socle $\pi(N)$ of N, i.e. by the set $\pi(N) \subset K(N)$ of prime divisors p of N, and an arbitrary divisor $\kappa \in K(N)$ is presented as a vector with integer components $0 \leq \alpha_p(\kappa) \leq \alpha_p(N)$, $p \in \pi(N)$, given by appropriate arithmetic exponents (see equation (A1.5)).

The action of the group C_N on the set $\tilde{N}$ of nodes of the magnet, determined by equation (4), is isomorphic with the additive action of the ring $\mathrm{End}\, C_N$, i.e. with the action of the additive group C_N of $\mathrm{End}\, C_N$ on the Brillouin zone B (equations (A2.6)-(A2.8)). Moreover, one defines the multiplicative action of the ring $\mathrm{End}\, C_N$ on the set $\tilde{N}$, given by equation (A2.18). Those endomorphisms $\eta_l \in \mathrm{End}\, C_N$ which

are invertible under multiplicative action (i.e. those for which $\text{lcd}(l, N) = 1$, so that l and N are mutually prime), form the Abelian group $\text{Aut}\, C_N$. A combination of the additive action of the ring $\text{End}\, C_N$ with the multiplicative action of the group $\text{Aut}\, C_N$ leads us in a natural way to the notion of holomorph $\text{Hol}\, C_N$ as the group given by equation (A2.20), and constituting a generalisation of the notion of a space group of a crystal. In this generalisation, the invariant subgroup

$$C_N \simeq \{(l, \eta_1) \,|\, l \in \tilde{N}\} \lhd \text{Hol}\, C_N \tag{12}$$

is the translation group of the crystal $\tilde{N}$, whereas the corresponding quotient group, i.e.

$$(\text{Hol}\, C_N)/C_N = \text{Aut}\, C_N \tag{13}$$

can be interpreted as the group of 'generalised rotations' of the crystal. Not all 'generalised rotations' have the meaning of isometry transformations of the crystal, but only those 'geometric automorphisms' which preserve or reverse the cyclic order on N. Evidently, the geometric automorphisms constitute (for $N > 2$) the two-element group $Q = \{\eta_1, \eta_{N-1}\} \lhd \text{Aut}\, C_N$ (see equation (A2.22)), which is an ordinary point group for the linear chain with the unit element η_1 and one-dimensional inversion η_{N-1} (see equation (A2.23)). An arbitrary automorphism $\eta_l \in \text{Aut}\, C_N$ determines (uniquely) a generator l of the group C_N, i.e. an element of order N in the additive group C_N of the ring $\text{End}\, C_N$ ($l \in \tilde{N}_1$ in the notation of equation (A2.24)). The action of the holomorph $\text{Hol}\, C_N$ on the crystal $\tilde{N}$, given formally by equation (A2.19), determines an embedding $\text{Hol}\, C_N \subset \Sigma_N$, constituting, according to equation (3), a covering of the embedding $C_N \subset \Sigma_N$ defined by equation (4). In the spirit of the prescription of Weyl, the permutations belonging to the holomorph $\text{Hol}\, C_N$ characterise all the invariant properties of our crystal $\tilde{N}$, whereas all other permutations of the symmetric group Σ_N break the symmetry of a linear chain.

It is natural in such a context to decompose the Brillouin zone B given by equation (6) into disjoint subsets B_κ given by equation (A2.28), constituting a generalisation of the notion of the star of a wavevector, known from the representation theory of space groups. Namely, the generalised star B_κ, $\kappa \in K(N)$, consists of all wavenumbers generated by the group $\text{Aut}\, C_N$ from the divisor $\kappa \in K(N) \subset B$. The number of elements $|B_\kappa|$ of this set is given by the value $\varphi(\bar{\kappa})$ of the Euler function φ (equation (A2.14)) for the complementary divisor $\bar{\kappa} = N/\kappa$ in the lattice $K(N)$. In particular, the generalised star

$$B_N = \{\kappa = N \equiv 0 \bmod N\} \tag{14}$$

is the centre of the Brillouin zone B, and for N even there exists the generalised star

$$B_{N/2} = \{\kappa = N/2\} \tag{15}$$

the boundary of B. Equation (A2.14) implies that these are the only one-element generalised stars. They coincide with ordinary stars for the linear chain, i.e. with orbits of the point group $Q \lhd \text{Aut}\, C_N$, given by equation (A2.22). All other ordinary stars consist of pairs $\{k, -k\} \subset B$ from 'interior' of the zone B. Thus a generalised star encloses, in general, several ordinary stars.

The principal property of the decomposition (A2.27) of the Brillouin zone B into generalised stars B_κ, $\kappa \in K(N)$, is the invariance of this decomposition under the action of the group $\text{Aut}\, C_N$, determined by the multiplicative action ζ of the ring $\text{End}\, C_N$ (equation (A2.26)). It results from the fact that, by definition, generalised stars B_κ are orbits of the group $\text{Aut}\, C_N$. We now observe that the lattice $K(N)$ of divisors of N

plays not only the important role of the lattice of subgroups of the translation group C_N, but also serves to classify generalised stars in the Brillouin zone.

The embedding $\mathrm{Hol}\, C_N \subset \Sigma_N$ implies a natural action of the holomorph $\mathrm{Hol}\, C_N$ (so that, in particular, $\mathrm{Aut}\, C_N \simeq \{(N, \eta_l)\,|\,\eta_l \in \mathrm{Aut}\, C_N\}$) in the space L of quantum states of the magnet, given by equation (7) as the subduction $P \downarrow \mathrm{Hol}\, C_N$, where P is the (linear) representation of Σ_N in L, defined by equation (10). Let L_k, $k \in B$, be the linear closure of all carrier spaces of the irreducible representation Γ_k of the group C_N in L, so that

$$L = \sum_{k \in B} \oplus L_k \tag{16}$$

is a unique decomposition of L into the direct sum of mutually orthogonal subspaces L_k and $\dim L_k = \rho(k)$. It is easy to observe that an evident invariance of the space L under the action P of the symmetric group Σ_N implies that each element $(N, \eta_l) \in \mathrm{Hol}\, C_N \subset \Sigma_N$ generates a permutation on the set $\{L_k \,|\, k \in B\}$ of subspaces invariant under C_N. In other words, the subduction $(P \downarrow \mathrm{Hol}\, C_N) \downarrow \mathrm{Aut}\, C_N$ generates the action γ of the group $\mathrm{Aut}\, C_N$ on the set $\{L_k \,|\, k \in B\}$, given by

$$\gamma(\eta_l) = \begin{pmatrix} L_k \\ L_{\psi(lk \bmod N)} \end{pmatrix} \qquad l \in \tilde{N} \qquad k \in B \tag{17}$$

where $\psi: \tilde{N} \to B$ is a bijection defined by equation (A2.7). It implies, together with equation (A2.26) that if one identifies the set $\{L_k \,|\, k \in B\}$ with the Brillouin zone B, then the action γ coincides simply with the action ζ of $\mathrm{Aut}\, C_N$ on B, defined in appendix 2. The fact that each $P(\sigma)$, $\sigma \in \Sigma_N$ (so, in particular, each $P(N, \eta_l)$, $\eta_l \in \mathrm{Aut}\, C_N$), is a non-singular operator implies that all spaces $L_{\psi(lk \bmod N)}$, generated from an arbitrary $k \in B$ by the group $\mathrm{Aut}\, C_N$, have the same dimension. We obtain, therefore, that for an arbitrary $\kappa \in K(N) \subset B$

$$\rho(k) \equiv \dim L_k = \text{constant} \qquad k \in B_\kappa \tag{18}$$

so that the density of states of the magnet is constant on each generalised star in the Brillouin zone. Thus this density depends effectively only on κ, i.e. it is a function $\omega: K(N) \to Z$ on the lattice $K(N)$ of divisors of N. It is perhaps the most important conclusion to be drawn from an application of Weyl's prescription for our case.

3. Interpretation of the analytical formula for the density of states

We proceed to study, in the spirit of Weyl's prescription, the structure of analytical expression for the density of states $\rho(k)$, $k \in B$, obtained in I. To this end, we will look at the derivation from a structural point of view, introducing some change in notation (in particular, our actual crucial divisors κ, κ_0, and κ' stand for the complementary divisors $\bar{\kappa}$, $\bar{\kappa}_0$ and $\bar{\kappa}'$ in I).

Character theory yields

$$\rho(k) = \frac{1}{N} \sum_{j \in \tilde{N}} \chi^P(\sigma_j) \exp(-2\pi i k j / N) \tag{19}$$

where $\chi^P(\sigma_j)$ is the character of the representation P for the element $\sigma_j \in C_N \subset \Sigma_N$, given by equation (4). The decomposition (A2.24) allows us to treat $j \in \tilde{N}_\kappa \subset C_N$ as a pair (κ, ξ), where $\kappa \in K(N)$ is a divisor of N and $\xi \in (\bar{\kappa})_1$, i.e. ξ is mutually prime

with the complementary divisor $\bar{\kappa}$ (see the notation of equation (A2.25)). In other words, an arbitrary $j \in \tilde{N}$ can be uniquely presented as a product

$$j = \xi\kappa \qquad \kappa \in K(N) \qquad \xi \in (\bar{\kappa})_1. \tag{20}$$

The character $\chi^P(\sigma_j)$ is given, due to some combinatorial arguments (see I), by the formula

$$\chi^P(\sigma_j) = \chi^P(\sigma_\kappa) = n^\kappa \qquad j \in \tilde{N}_\kappa \tag{21}$$

so that it is constant on each subset $\tilde{N}_\kappa \subset C_N$, $\kappa \in K(N)$, i.e. on classes of the group C_N with respect to the action of the group $\mathrm{Aut}\, C_N$ (i.e. on equivalents of generalised stars in the 'real space'). Similarly, the decomposition (A2.27) of the Brillouin zone B into generalised stars yields the presentation

$$k = \psi(\xi_0\kappa_0) \qquad \kappa_0 \in K(N) \qquad \xi_0 \in (\bar{\kappa}_0)_1 \tag{22}$$

with ψ given by equation (A2.7). As a result, we rewrite equation (19) in the form

$$\rho(k) \equiv \rho(\xi_0\kappa_0) = \frac{1}{N} \sum_{\kappa \in K(N)} n^\kappa \sum_{\xi \in (\bar{\kappa})_1} \exp(2\pi i \xi \xi_0 \kappa\kappa_0/N) \tag{23}$$

with separation of the sum over the group C_N into two sums: over elements κ of the lattice $K(N)$ and, for each $\kappa \in K(N)$, over $\xi \in (\bar{\kappa})_1$ (such that $\xi\kappa \in \tilde{N}_\kappa$).

The sum over ξ in equation (23) constitutes a sum of primary roots of degree $\bar{\kappa}' = N/\kappa'$ from unity, with

$$\kappa' = \mathrm{lcd}(\kappa\kappa_0, N). \tag{24}$$

Evaluation of this sum is structurally associated with the multiplicative action (A2.18) of the ring $\mathrm{End}\, C_N$ on the set $\tilde{N}$ (i.e. also on the group C_N). Using equations (20) and (22) we can write down this action in a form

$$\eta_{\xi_0\kappa_0} = \begin{pmatrix} \xi\kappa \\ \xi'\kappa' \end{pmatrix} \qquad \kappa_0 \in K(N) \qquad \xi_0 \in (\bar{\kappa}_0)_1 \qquad \kappa \in K(N) \qquad \xi \in (\bar{\kappa})_1 \tag{25}$$

where $\kappa' \in K(N)$ is given by equation (24) and $\xi' = \xi_0\xi \bmod \bar{\kappa}' \in (\bar{\kappa}')_1$. Each endomorphism $\eta_l : C_N \to C_N$ thus carries a class $\tilde{N}_\kappa$, $\kappa \in K(N)$, into the class $\tilde{N}_{\kappa'}$, $\kappa' = \mathrm{lcd}(\kappa\kappa_0, N)$, such that the restriction $\eta_l|_{\tilde{N}_\kappa}$ is a surjection in which the counterimage of an arbitrary element $\xi'\kappa' \in \tilde{N}_{\kappa'}$ consists of $\varphi(\bar{\kappa})/\varphi(\bar{\kappa}')$ elements of the class $\tilde{N}_\kappa$. Moreover, each pair of endomorphisms $(\eta_l, \eta_{l'})$ from a class $\tilde{N}_{\kappa_0}$ (i.e. $l = \xi_0\kappa_0$ and $l' = \xi_0'\kappa_0'$, or, equivalently, $k = \psi(l) \in B_{\kappa_0}$ and $k' = \psi(l') \in B_{\kappa_0}$) carry a given class $\tilde{N}_\kappa$ into the same class $\tilde{N}_{\kappa'}$ and differ only up to modulo an action within the class $\tilde{N}_{\kappa'}$.

The multiplicative action of the ring $\mathrm{End}\, C_N$ on the group C_N thus generates the action of the lattice $K(N)$ on itself in a natural way, i.e. the mapping $\beta : K(N) \to \mathrm{Map}\, K(N)$ ($\equiv \{u : K(N) \to K(N)\} = K(N)^{K(N)}$), given by

$$\beta(\kappa_0) = \begin{pmatrix} \kappa \\ \mathrm{lcd}(\kappa\kappa_0, N) \end{pmatrix} \qquad \kappa_0 \in K(N) \qquad \kappa \in K(N). \tag{26}$$

In particular, we have the implications

$$(\alpha_p(\kappa) + \alpha_p(\kappa_0) \leq \alpha_p(N) \qquad p \in \pi(N)) \Rightarrow \kappa' = \kappa\kappa_0 \tag{27}$$

$$(\alpha_p(\kappa) + \alpha_p(\kappa_0) \geq \alpha_p(N) \qquad p \in \pi(N)) \Rightarrow \kappa' = N. \tag{28}$$

In general, the action β of the lattice $K(N)$ on itself can be looked at as a displacement of its elements towards the maximal divisor N. This displacement becomes more obvious by rewriting equation (24), determining the action β, in the form

$$\kappa' = \mathrm{lcd}(\kappa\kappa_0, \kappa\bar{\kappa}) \equiv \kappa\,\mathrm{lcd}(\kappa_0, \bar{\kappa}) \tag{29}$$

corresponding (complementarily) to equation (A14) of I.

The sum over ξ in equation (23) is associated with the restriction $\eta_l|_{\bar{N}_\kappa}$, $l = \xi_0\kappa_0$. Simple arguments from number theory (Narkiewicz 1977, Hasse 1979), in particular those related to cyclotomic polynomials (Foulkes 1972) yield

$$\sum_{\xi\in(\bar{\kappa})_1} \exp(2\pi\mathrm{i}\xi\xi_0\kappa\kappa_0/N) = \frac{\varphi(\bar{\kappa})}{\varphi(\bar{\kappa}')}\mu(\bar{\kappa}') \tag{30}$$

independently on $\xi_0 \in (\bar{\kappa}_0)_1$.

Let $\omega: K(N) \to Z$ be the mapping determined by

$$\omega(\kappa_0) = \sum_{\kappa\in K(N)} \omega_\kappa(\kappa_0) \qquad \kappa_0 \in K(N) \tag{31}$$

where

$$\omega_\kappa(\kappa_0) = \frac{n^\kappa}{N}\frac{\varphi(\bar{\kappa})}{\varphi(\bar{\kappa}')}\mu(\bar{\kappa}') \qquad \kappa' = \mathrm{lcd}(\kappa\kappa_0, N). \tag{32}$$

Then the desired expression for the density of states for the linear magnetic chain in the Brillouin zone can be written in the form

$$\rho(k) = \omega(\kappa_0) \qquad k \in B_{\kappa_0} \subset B \tag{33}$$

reflecting all invariant properties of this density. In particular, this form displays explicitly that the density is constant on each generalised star B_{κ_0} in the Brillouin zone B, and, moreover, equation (32) relates this density to the action β of the lattice $K(N)$ of divisors of N on itself, as given in equation (26).

4. A discussion of the density of states

The total density of states can be naturally decomposed into the sum of contributions ω_κ, $\kappa \in K(N)$, according to equations (31)-(32), so that the contribution classified by a particular divisor $\kappa \in K(N)$ is proportional to n^κ/N, and the 'weight' of this contribution, given by equation (30), is constant on each generalised star B_{κ_0} in the Brillouin zone and depends on the element $\kappa' \in K(N)$, given by equation (24). The distribution of states in the Brillouin zone is thus determined essentially by the action β of the lattice $K(N)$ on itself, with a mapping $\beta(\kappa_0)$, $\kappa_0 \in K(N) \subset B$, carrying the class $\tilde{N}_\kappa$, $\kappa \in K(N) \subset C_N$, into the class $\tilde{N}_{\kappa'}$.

The main contribution corresponds to the maximal divisor $\kappa = N$ and is given by

$$\omega_N(\kappa_0) = n^N/N \qquad \kappa_0 \in K(N) \subset B \tag{34}$$

so that it is homogeneous within the whole Brillouin zone. It thus provides a homogeneous background, on which corrections appear in a form of several distributions of condensations and holes, associated with the other divisors of the lattice $K(N)$. As shown in I, the corrections ω_κ, $\kappa \neq N$, for N large enough, become very small in comparison with the background ω_N.

The presence of the Mobius function in equation (32) yields an additional selection rule, which provides vanishing of values $\omega_\kappa(\kappa_0)$ for some contributions ω_κ at some generalised stars $B_{\kappa_0} \subset B$. Namely, the value $\mu(\kappa)$ of the Mobius function becomes zero on the whole lattice $K(N)$ with the exception of all divisors κ which are the nodes adjacent to the elementary cell of the hyperparallelepiped $K(N)$, spanned on the socle $\pi(N)$. Simple combinatoric considerations associated with the geometric presentation of the lattice $K(N)$ yield a 'cut-off' of contributions corresponding to generalised stars outside some vicinity of the maximal divisor $\kappa_0 = N$ in the hyperparallelepiped $K(N)$. We can discuss briefly (although somehow vaguely) a cut-off from the long-wave side. To formulate this cut-off exactly, let us consider a contribution ω_κ for a fixed $\kappa \in K(N)$ and let $\kappa_{0\min} \in K(N) \subset B$ be given in terms of arithmetic exponents as

$$\alpha_p(\kappa_{0\min}) = \left\{ \begin{array}{ll} \alpha_p(\bar{\kappa}) - 1 & \text{for } \alpha_p(\bar{\kappa}) \geq 1 \\ 0 & \text{otherwise} \end{array} \right\} p \in \pi(N). \tag{35}$$

Then the non-vanishing values $\omega_\kappa(\kappa_0)(\neq 0)$ result only for

$$\kappa_0 \in [\kappa_{0\min}, N]. \tag{36}$$

In the geometric presentation of the lattice $K(N)$, the segment $[\kappa_{0\min}, N]$ has such a shape that it encloses the complementary divisor $\bar{\kappa} \in K(N)$ together with all its nearest neighbours 'from the bottom', so that $\kappa_{0\min}$ is the minimal element of this segment.

In particular, for $\kappa \in [\bar{\kappa}_e, N]$ (see equation (A1.7)), i.e. for the segment constituting the elementary cell of the hyperparallelepiped $K(N)$ spanned on the cosocle $\bar{\pi}(N)$, we obtain $\kappa_{0\min} = 1$, so that the cut-off becomes ineffective, and thus the corresponding contributions are distributed over the whole Brillouin zone (inhomogeneously, with the exception of $\kappa = N$). All other contributions do not vanish only for some distinguished generalised stars B_{κ_0}, namely for those which satisfy the selection rule (36) on the lattice $K(N)$. Moreover, we have

$$\bigcup_{\kappa_0 \in [\kappa_{0\min}, N]} B_{\kappa_0} \simeq C_{\bar{\kappa}_{0\min}} \tag{37}$$

i.e. the union of classes corresponding to generalised stars yielding non-vanishing values of the contribution ω_κ forms the subgroup $C_{\bar{\kappa}_{0\min}}$ of C_N, generated by the divisor $\kappa_{0\min}$. The distribution of the corresponding condensations or holes therefore display a discontinuous nature: all these points constitute a 'subzone' $C_{\bar{\kappa}_{0\min}}$ in the (finite) Brillouin zone B, with the 'lattice constant' (i.e. the distance of nearest neighbours in the subzone $C_{\bar{\kappa}_{0\min}}$ imposed by the cyclic order in the zone B) given by $\kappa_{0\min}$, and the total number of points given by the complementary divisor $\bar{\kappa}_{0\min}$.

It is worthwhile to observe that the definitely discontinuous character of the distribution of condensations and holes in the Brillouin zone can be attributed to a disagreement between the 'natural' order in the set of integers determining the cyclic order in the Brillouin zone given by equation (6) and the partial order in the lattice $K(N)$ of divisors of N. As a result, the decomposition (A2.27) of the Brillouin zone B into generalised stars B_{κ_0} becomes, except for trivial cases, a decomposition into subsets which are 'rarefied' in B, i.e. each pair (k, k'), $k \in B_{\kappa_0}$, $k' \in B_{\kappa_0}$, of wavenumbers of a given generalised star B_{κ_0} is separated in B by some wavenumbers belonging to other stars. A similar remark applies to the decomposition (A2.24) of the crystal $\tilde{N}$ into classes $\tilde{N}_\kappa$, $\kappa \in K(N)$. It seems to us that such rarefied subsets constitute a characteristic feature of the finiteness of the linear chain.

Within the subzone $C_{\bar{\kappa}_{0\min}} \subset B$, defined by the contribution ω_κ, the Mobius function differentiates generalised stars $B_{\kappa_0} \subset C_{\bar{\kappa}_{0\min}}$ into those corresponding to condensations of states ($\mu(\bar{\kappa}') = 1$) and holes ($\mu(\bar{\kappa}') = -1$). Due to a sum rule

$$\sum_{\kappa_0 \in K(N)} \varphi(\kappa_0)\omega_\kappa(\kappa_0) = n^N \delta_{\kappa,N} \tag{38}$$

each contribution ω_κ, $\kappa \neq N$, is a balanced distribution of condensations and holes on the homogeneous background ω_N.

The centre of the Brillouin zone, i.e. the generalised star $B_N = \{k = 0 \equiv N \bmod N\}$ is associated with the highest condensation of states as the intersection of all subgroups $C_{\bar{\kappa}_{0\min}}$ of the group C_N. We obtain for this case

$$\rho(0) = \frac{1}{N} \sum_{\kappa \in K(N)} n^\kappa \varphi(\bar{\kappa}) = \max\{\rho(k) | k \in B\}. \tag{39}$$

The centre is the nearest neighbour (in the cyclic order) of wavenumbers $k = \pm 1 \in B_1$, where

$$\rho(\pm 1) = \frac{1}{N} \sum_{\kappa \in K(N)} n^\kappa \mu(\bar{\kappa}) = \min\{\rho(k) | k \in B\} \tag{40}$$

so that the generalised star B_1 is associated with the maximal number of holes in B. For N even, the density for the boundary $B_{N/2} = \{k = N/2\}$ is

$$\rho(N/2) = \frac{1}{N} \sum_{\kappa \in K(N)} (-n)^\kappa \varphi(\bar{\kappa}). \tag{41}$$

We also quote some special cases in detail in order to demonstrate some characteristic features of inhomogeneities of the density ρ. The contributions $\omega_{\bar{p}}$, corresponding to the coatom $\bar{p} = N/p$ of the lattice $K(N)$, take on a very simple form, given by

$$\omega_{\bar{p}}(\kappa_0) = \frac{n^{N/p}}{N} \times \begin{cases} p - 1 & \text{if } \mathrm{ldc}(\kappa_0, p) = p \\ -1 & \text{otherwise} \end{cases} \tag{42}$$

so that they describe the (homogeneous) distribution of condensations for all those wavenumbers $k \in B$, which are multiplicities of p, together with homogeneous compensating distributions of holes for all other wavenumbers in the Brillouin zone. The total number of states involved in the contribution $\omega_{\bar{p}}$ is zero, in agreement with the general formula (38). In particular, for N even there exists the coatom $\bar{p} = N/2$, for which

$$\rho_{N/2}(k) = (-1)^k n^{N/2}/N. \tag{43}$$

This corresponds to the term $\kappa = N/2$ in the sum in equation (41), and describes a 'homogeneously alternating' distribution of condensations (k even) and holes (k odd).

For $\bar{\kappa} = p^\alpha$ we obtain

$$\omega_{N/p^\alpha}(\kappa_0) = \frac{n^{N/p^\alpha}}{N} \times \begin{cases} p^{\alpha-1}(p-1) & \text{for } \alpha_p(\kappa_0) \geq \alpha \\ -p^{\alpha-1} & \text{for } \alpha_p(\kappa_0) = \alpha - 1 \\ 0 & \text{otherwise.} \end{cases} \tag{44}$$

This contribution differs from zero only for some generalised stars, $B_{\kappa_0} \subset C_{\bar{\kappa}_{0\min}}$, where $\kappa_{0\min}$ is given by equation (35), and corresponds to a distribution of holes over each $k \in B$ which is divisible exactly by $p^{\alpha-1}$, together with the compensating condensations for each $k \in B$ which is divisible by higher powers of p. For all other $k \in B$ this contribution vanishes. Equation (32), together with formulae (A1.18) and (A2.14), provides an easy derivation of similar more extended formulae for other special cases.

5. An example

We proceed to illustrate our calculations on an example:

$$N = 90 = 2 \times 3^2 \times 5 \qquad \pi(N) = \{2, 3, 5\}. \qquad (45)$$

The lattice of divisors $K(90)$ is presented in figure 1. The decomposition of the Brillouin zone

$$B = \{0, \pm 1, \pm 2, \ldots, \pm 44, 45\} \qquad (46)$$

into generalised stars is given in table 1. A comparison of the first column of this table, where divisors $\kappa \in K(90)$ are ordered according to the natural order implied by the embedding $K(90) \subset Z$, with figure 1 yields an imagination of the difference between the cyclic order in the linear chain $\tilde{N}$ and the partial order in the lattice $K(N)$ imposed by atoms p of the socle $\pi(N)$. A brief glance at the last column illustrates the meaning
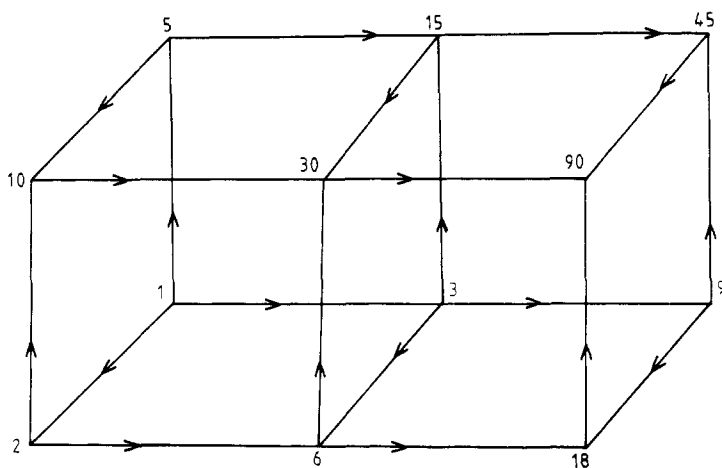
Figure 1. A geometric picture of the lattice $K(90)$. The nodes 2, 3 and 5 are the atoms of the lattice, and 45, 30 and 18 are the corresponding coatoms. Arrows indicate the partial order.

Table 1. Decomposition of the Brillouin zone into generalised stars for $N = 90$.

κ	$\bar{\kappa}$	$\varphi(\bar{\kappa})$	B_κ
1	90	24	$\pm 1, \pm 7, \pm 11, \pm 13, \pm 17, \pm 19, \pm 23, \pm 29, \pm 31, \pm 37, \pm 41, \pm 43$
2	45	24	$\pm 2, \pm 4, \pm 8, \pm 14, \pm 16, \pm 22, \pm 26, \pm 28, \pm 32, \pm 34, \pm 38, \pm 44$
3	30	8	$\pm 3, \pm 21, \pm 33, \pm 39$
5	18	6	$\pm 5, \pm 25, \pm 35$
6	15	8	$\pm 6, \pm 12, \pm 24, \pm 42$
9	10	4	$\pm 9, \pm 27$
10	9	6	$\pm 10, \pm 20, \pm 40$
15	6	2	± 15
18	5	4	$\pm 18, \pm 36$
30	3	2	± 30
45	2	1	45 (the boundary)
90	1	1	$90 \equiv 0 \bmod 90$ (the centre)

Table 2. The density $\omega_\kappa(\kappa_0)$ for $N = 90$ in units of n^κ/N.

κ/κ_0	1	2	3	5	6	9	10	15	18	30	45	90
1	0	0	-3	0	3	6	0	12	-6	-12	-24	24
2	0	0	3	0	3	-6	0	-12	-6	-12	24	24
3	-1	1	2	4	-2	2	-4	-8	-2	8	-8	8
5	0	0	3	0	-3	-6	0	3	6	-3	-6	6
6	1	1	-2	-4	-2	-2	-4	8	-2	8	8	8
9	4	-1	4	-4	-1	4	4	-4	-1	4	-4	4
10	0	0	-3	0	-3	6	0	-3	6	-3	6	6
15	2	-1	-2	2	2	-2	-1	-2	2	2	-2	2
18	-1	-1	-1	4	-1	-1	4	4	-1	4	4	4
30	-1	-1	2	-1	2	2	-1	2	2	2	2	2
45	-1	1	-1	-1	1	-1	1	-1	1	1	-1	1
90	1	1	1	1	1	1	1	1	1	1	1	1

of generalised stars as some 'rarefied' subsets of the set (46): each pair of nearest neighbours (in the cyclic order) in a generalised star B_κ, $\kappa \in K(90)$, are separated in B by at least one element of another generalised star.

The results for the density of states are given in table 2. The last row of this table corresponds to the homogeneous contribution ω_{90} (equation (34)), and the next to last to the homogeneously alternating contribution ω_{45} (equation (43)), labelled by the coatom $\bar\kappa = 45$ of the atom $\kappa = 2$. All those contributions ω_κ which are spread over the whole Brillouin zone (i.e. $\omega_\kappa(\kappa_0) \neq 0$, $\kappa_0 \in K(90)$) correspond to the segment

$$[30, 90] = \{3, 6, 9, 15, 18, 30, 45, 90\} \tag{47}$$

spanned over the cosocle $\bar\pi(90) = \{45, 30, 18\}$. The remaining part of the lattice $K(90)$ also forms a segment in this case (accidentally), namely

$$[1, 10] = \{1, 2, 5, 10\}. \tag{48}$$

The contributions ω_κ, $\kappa \in [1, 10]$ do not vanish (i.e. $\omega_\kappa(\kappa_0) \neq 0$) only for $\kappa_0 \in [30, 90]$, i.e. for the right-hand side elementary cube in figure 1. This numerical result of table 2 is in agreement with the general formula (35), which yields the minimal element

$$\kappa_{0\,\mathrm{min}} = 2^0 \times 3^1 \times 5^0 = 3 \tag{49}$$

of the segment $[\kappa_{0\,\mathrm{min}}, 90]$ for each $\kappa \in [1, 10]$.

6. Final remarks and conclusions

In this paper we have discussed some invariant properties of the density of states in the Brillouin zone for the model of a one-dimensional Heisenberg magnet consisting of N spins s arranged to form a linear chain. A detailed study of the analytical expression for this density, given in I, and some physical interpretation of the mathematical notions involved in the derivation of this expression provide an insight into the structure of the inhomogeneities of this density. We have also demonstrated that such a study and physical interpretation constitute a particular example of realisation of a general Weyl prescription for the determination of the invariant properties of mathematical models with a given symmetry.

In our case, the symmetry of the problem with respect to the group Aut C_N of all automorphisms of the cyclic group C_N, determining the geometric distribution of nodes

of the magnet, implies that the density of states is constant on generalised stars, i.e. on some rarefied subsets of the discrete Brillouin zone B, constituting orbits of the action of Aut C_N on B. All the details of the distribution of inhomogeneities of the density of states are determined by selection rules on the lattice $K(N)$ of divisors of N, being also the lattice of subgroups of the group C_N. According to the above description, one can expect that a breaking of translational symmetry of the linear chain, e.g. by an admixture, vacancy, etc, should yield a modulation of the density of states within a generalised star (the density should then be defined as an appropriate quantum mean value, since the wavenumbers $k \in B$ cease to be exact quantum numbers).

We hope that our paper clearly justifies an important role for the arithmetic structure of the integer N (prime divisors, lattices, the socle, coatoms, segments, etc) in an invariant description of the physical properties of models with a finite number N of (identical) constituent parts. Our approach is essentially an application of ancient notions like Erastothenes' sieve for a classification of states of the quantum model of the Heisenberg magnet. Description of this approach in terms of Weyl's prescription ensures the manifest invariance of this description. It is helpful to overcome objections associated with some floating opinions that the 'physical' properties of a model of a linear magnet should not depend upon the arithmetic structure of N (at least for N large enough) because of an irregular variation of the details of this structure under the variation of N. In this context, it is worthwhile to mention that, independently from a really irregular change in the details of the arithmetic structure of N, there remains a common feature for an arbitrary N, namely the decomposition of the discrete Brillouin zone into disjoint subsets, each having a form of being 'selected by a sieve', i.e. a rarefied subset of the full zone. Such subsets, appearing strange to someone used to a functional analysis operating with the notion of continuity, seem for us to be a characteristic feature of an adequate description of finite systems.

Inhomogeneity of the density of states becomes relatively small for large N due to the power law n^κ (see equation (32)). If it happened, however, that a rarefied band was lying low enough in the energy scale, then such a band would lead to a (crystal) sublattice with the period κ being an element of the (mathematical) lattice $K(N)$. For κ large enough such a modulation could characterise some incommensurate phases of a crystal, resembling incommensurate phases known from recent literature (Bak 1982).

The problem of the decomposition of the permutation representation P into irreducible representations Γ_k of the group C_N, considered in the present paper, can be looked at as one of the questions covered by the Racah-Wigner calculus (Biedenharn and Louck 1968, 1981 and references therein), in particular with respect to permutation representations (Lulek 1985a,b). The solution proposed in this paper can be placed at the level of irreducible representations of the translation group of the crystal. From the physical point of view it would be interesting to point out some further good quantum numbers classifying the states with a given wavenumber k. We hope to approach such results by way of an appropriate application of Racah-Wigner calculus for transitive representations at the level of irreducible bases.

Appendix 1. The lattice of subgroups of a cyclic group

Let

$$N = \prod_{p \in \pi(N)} p^{\alpha_p(N)} \tag{A1.1}$$

be the canonical decomposition of an integer N into prime factors. Each prime integer p entering non-trivially into the decomposition (A1.1) (i.e. with positive arithmetic exponent $\alpha_p(N) > 0$) is referred to (in algebra) as an atom of N and the set $\pi(N)$ of all atoms of N as the socle of N (Kasch 1977, Grätzer 1978, Rybnikov 1972).

Consider the set of all subgroups of the cyclic group C_N. Each element of this set is a cyclic group C_κ, with the order κ equal to a divisor of N. This set, together with the relation of partial order defined by the inclusion, forms the so-called lattice (not to be confused with a crystal lattice), i.e. a partially ordered set with unique minimal element C_1 and maximal C_N. Elements of the lattice of subgroups of C_N can thus be uniquely classified by the set (lattice)

$$K(N) = \{\kappa \in \tilde{N} \,|\, \mathrm{lcd}(\kappa, N) = \kappa\} \tag{A1.2}$$

of all divisors of N, with $\mathrm{lcd}(\kappa, N)$ denoting the largest common divisor of integers κ and N.

The subset

$$K_p(N) = \{\kappa \in K(N) \,|\, \kappa = p^{\alpha_p(\kappa)}, 0 \le \alpha_p(\kappa) \le \alpha_p(N)\} \subset K(N) \tag{A1.3}$$

of the lattice $K(N)$ of divisors of N encloses primary subgroups of C_N, i.e. subgroups of the order of a power of an atom $p \in \pi(N)$. Primary subgroups are distinguished in $K(N)$ by the fact that the relation of inclusion defines in each $K_p(N)$, $p \in \pi(N)$, the linear (not only partial) order and, moreover, none of primary subgroups can be presented as the direct product of its non-trivial subgroups. Instead, if $\kappa_1 \in K_{p_1}(N)$, $\kappa_2 \in K_{p_2}(N)$, $p_1 \neq p_2$, then $C_{\kappa_1} \otimes C_{\kappa_2} \simeq C_{\kappa_1 \kappa_2}$ is a subgroup of C_N (i.e. $\kappa_1 \kappa_2 \in K(N)$). These features yield a nice geometric presentation of the partial order in the lattice $K(N)$ (Rybnikov 1972, Lulek and Lulek 1987). Namely, the lattice $K(N)$ can be expressed as the cartesian product

$$K(N) = \prod_{p \in \pi(N)} \times K_p(N) \tag{A1.4}$$

so that an arbitrary divisor $\kappa \in K(N)$ is presented by a sequence of its arithmetic exponents

$$\kappa = \prod_{p \in \pi(N)} p^{\alpha_p(\kappa)} \equiv (\ldots \alpha_p(\kappa) \ldots) \tag{A1.5}$$

corresponding to all atoms of the socle $\pi(N)$. Thus, interpreting the divisors κ as vectors (with integer components given by arithmetic exponents $\alpha_p(\kappa)$, $p \in \pi(N)$) in a $|\pi(N)|$-dimensional linear space over the field R, equipped with an orthonormal basis labelled by atoms of the socle $\pi(N)$, we obtain a picture of the lattice $K(N)$ as

a hyperparallelepiped with edges determined by linearly ordered sets $K_p(N)$. The prime divisors

$$\kappa = p = (0, \ldots, 1, \ldots, 0) \qquad p \in \pi(N) \tag{A1.6}$$

with the unity in a place corresponding to the atom p and zero otherwise, are vectors of an orthonormal basis in this space, whereas the divisor

$$\kappa_e = \prod_{p \in \pi(N)} p = (1, \ldots, 1) \tag{A1.7}$$

associated with the socle $\pi(N)$ is the maximal element of the hypercubic 'elementary cell'. Thus the lattice $K(N)$ constitutes, in this picture, a finite hypercubic lattice spanning the hyperparallelepiped. In particular, the number of elements of the lattice $K(N)$ is

$$|K(N)| = \prod_{p \in \pi(N)} (\alpha_p(N) + 1). \tag{A1.8}$$

The partial order in the lattice $K(N)$ is presented by straight lines connecting the nearest neighbours in the hypercubic lattice, equipped with such a direction that the projection of each line into the direction of the main diagonal κ_e given by equation (A1.7) is positive. Then the relation of inclusion $\kappa_1 \subset \kappa_2$ (i.e. $C_{\kappa_1} \lhd C_{\kappa_2}$) holds for all such pairs $(\kappa_1, \kappa_2) \in K(N) \times K(N)$, for which there exists a chain of lines with each link directed from κ_1 to κ_2. One also assumes $\kappa \subseteq \kappa$, $\kappa \in K(N)$. In this picture the divisors κ are nodes, and oriented lines connecting the nearest neighbours are edges of a transmission circuit with the minimal element $\kappa = 1 = (0, \ldots, 0)$ and maximal element $\kappa = N = (\ldots \alpha_p(N) \ldots)$ playing the role of input and output respectively, with the orientation of the lines being the direction of transmission.

Each divisor $\kappa \in K(N)$ is associated with the complementary divisor

$$\bar{\kappa} = N/\kappa \tag{A1.9}$$

which also belongs to $K(N)$. In particular, $\bar{p} = N/p$ is referred to as a coatom of N, and the set $\bar{\pi}(N) = \{\bar{p} \mid p \in \pi(N)\}$ is the cosocle. Geometrically, the complementary divisor $\bar{\kappa}$ can be obtained by an inversion of κ in the centre of the hyperparallelepiped (this centre is not necessarily an element of $K(N)$).

An important notion in the theory of lattices is that of a segment, i.e. essentially a kind of subset constituting a new lattice itself with respect to the assumed partial order. Let $\kappa_1 \in K(N)$, $\kappa_2 \in K(N)$ and $\kappa_1 \subseteq \kappa_2$. A segment $[\kappa_1, \kappa_2]$ is a lattice

$$[\kappa_1, \kappa_2] = \{\kappa \in K(N) \mid \kappa_1 \subseteq \kappa \subseteq \kappa_2\} \simeq K(\kappa_2/\kappa_1). \tag{A1.10}$$

Moreover, for $\kappa_1 \not\subseteq \kappa_2$ one assumes $[\kappa_1, \kappa_2] = \varnothing$, the empty set. Evidently, κ_1 and κ_2 are minimal and maximal elements of the segment $[\kappa_1, \kappa_2]$ respectively. Geometrically, the segment $[\kappa_1, \kappa_2] \subset K(N)$, $\kappa_1 \subseteq \kappa_2$, corresponds to a subhyperparallelepiped in $|\pi(\kappa_2/\kappa_1)| \leqslant |\pi(N)|$ dimensions, uniquely determined by the extremal elements κ_1 and κ_2. In particular, if $[\kappa_1, \kappa_2] = \{\kappa_1, \kappa_2\}$, i.e. for a segment consisting of exactly two elements, one has $|\pi(\kappa_2/\kappa_1)| = 1$, i.e. the subhyperparallelepiped reduces to the line connecting κ_1 with κ_2, parallel to the edge corresponding to the atom $p = \kappa_2/\kappa_1$. Then κ_2 is obviously a nearest neighbour of κ_1 towards the maximal element N, and one says that κ_2 covers κ_1. The segment $[\kappa, \kappa] = \{\kappa\}$, $\kappa \in K(N)$ is a trivial lattice, consisting of one element.

It is possible to determine uniquely the minimal segment enclosing two arbitrary divisors $\kappa_1 \in K(N)$ and $\kappa_2 \in K(N)$ (they can be incomparable by the partial order in

$K(N)$). To this aim, one introduces two binary operations on $K(N)$: the intersection $\wedge : K(N) \times K(N) \to K(N)$, given by

$$\kappa_1 \wedge \kappa_2 = \mathrm{lcd}(\kappa_1, \kappa_2) \qquad \kappa_1 \in K(N) \qquad \kappa_2 \in K(N) \qquad (A1.11)$$

and the union $\vee : K(N) \times K(N) \to K(N)$, given by

$$\kappa_1 \vee \kappa_2 = \mathrm{lcm}(\kappa_1, \kappa_2)$$

$$\equiv \kappa_1 \kappa_2 / \mathrm{lcd}(\kappa_1, \kappa_2) \qquad \kappa_1 \in K(N) \qquad \kappa_2 \in K(N) \qquad (A1.12)$$

where $\mathrm{lcm}(\kappa_1, \kappa_2)$ denotes the least common multiple of κ_1 and κ_2. The minimal segment in $K(N)$, enclosing κ_1 and κ_2 is $[\mathrm{lcd}(\kappa_1, \kappa_2), \mathrm{lcm}(\kappa_1, \kappa_2)]$, with the intersection and union as the minimal and maximal elements, respectively.

We proceed to describe the role of the Mobius function in the lattice $K(N)$. Let us consider the set $\{f : K \times K \to Z\}$ of all functions on the cartesian product of an arbitrary lattice K by itself with integral values. This set, equipped with pointwise addition

$$(f_1 + f_2)(\kappa_1, \kappa_2) = f_1(\kappa_1, \kappa_2) + f_2(\kappa_1, \kappa_2) \qquad \kappa_1 \in K \qquad \kappa_2 \in K \qquad (A1.13)$$

and multiplication given by

$$(f_1 f_2)(\kappa_1, \kappa_2) = \sum_{\kappa_3 \in [\kappa_1, \kappa_2]} f_1(\kappa_1, \kappa_3) f_2(\kappa_3, \kappa_2) \qquad \kappa_1 \in K \qquad \kappa_2 \in K \qquad (A1.14)$$

becomes an algebra, called the algebra of incidences on K (Hall 1967, Rybnikov 1972, Satschkov 1977, Grätzer 1978). In particular, the zeta function ζ, defined by

$$\zeta(\kappa_1, \kappa_2) = \begin{cases} 1 & \text{if } \kappa_1 \subseteq \kappa_2 \\ 0 & \text{otherwise} \end{cases} \qquad (A1.15)$$

is an element of this algebra. The Mobius function $\bar{\mu} : K \times K \to Z$ is the function reciprocal to the zeta function in the algebra of incidences on the lattice K, i.e. $\zeta \bar{\mu} = \bar{\mu} \zeta = 1$, or

$$\sum_{\kappa_3 \in [\kappa_1, \kappa_2]} \bar{\mu}(\kappa_1, \kappa_3) = \begin{cases} 1 & \text{if } \kappa_1 = \kappa_2 \\ 0 & \text{otherwise.} \end{cases} \qquad (A1.16)$$

This formula allows us to determine recursively the Mobius function for an arbitrary lattice K. In the case of $K(N)$ we have

$$\bar{\mu}(\kappa_1, \kappa_2) = \begin{cases} \mu(\kappa_2/\kappa_1) & \text{for } \kappa_1 \subseteq \kappa_2 \\ 0 & \text{otherwise} \end{cases} \qquad (A1.17)$$

where $\mu : Z \to Z$ is a standard, single-argument Mobius function for the theory of numbers, given by

$$\mu(N) = \begin{cases} 1 & \text{for } N = 1 \\ (-1)^{|\pi(N)|} & \text{if } 0 \leqslant \alpha_p(N) \leqslant 1, p \in \pi(N) \\ 0 & \text{otherwise.} \end{cases} \qquad (A1.18)$$

Thus the support of the restriction of the standard Mobius function μ to the lattice $K(N) \subset Z$ consists of all these nodes of the parallelepiped $K(N)$, which have all components (arithmetic exponents) equal to zero or one, i.e. of all nodes adjacent to the elementary cell spanned on the socle $\pi(N)$.

Appendix 2. The ring of endomorphisms of a cyclic group

The ring

$$\text{End } C_N = \{\eta_l \,|\, l \in \tilde{N}\} \tag{A2.1}$$

consists of endomorphisms $\eta_l : C_N \to C_N$, $l \in \tilde{N}$, determined by the formula

$$\eta_l(j) = l \bmod N \qquad j \in \tilde{N} \tag{A2.2}$$

with the pointwise addition and the composition of mappings as the multiplication. We thus have

$$\eta_l + \eta_{l'} = \eta_{(l+l') \bmod N} \qquad l \in \tilde{N} \qquad l' \in \tilde{N} \tag{A2.3}$$

$$\eta_l \eta_{l'} = \eta_{l'} \eta_l = \eta_{(ll') \bmod N} \qquad l \in \tilde{N} \qquad l' \in \tilde{N} \tag{A2.4}$$

so that the ring $\text{End } C_N$ is isomorphic to the ring Z_N of remainders modulo N:

$$\text{End } C_N \simeq Z_N = (\tilde{N}, \text{`+' } \bmod N, \text{`·' } \bmod N) \tag{A2.5}$$

with the canonical isomorphism $\lambda : Z_N \to \text{End } C_N$ given by $\lambda(l) = \eta_l$, $l \in \tilde{N}$.

The additive group

$$C_N^* = \lambda(\tilde{N}, \text{`+' } \bmod N) \tag{A2.6}$$

of the ring $\text{End } C_N$ is called the dual group to the group C_N (Lang 1970, § 11). Although C_N and C_N^* are mutually isomorphic as abstract groups (with the isomorphism λ), it is convenient to distinguish them in crystallography by attaching different meanings to carrier sets of their regular representations: the orbit $\tilde{N}$ of C_N, given by equation (4), defines the set of nodes of the crystal in 'real space', whereas the orbit of C_N^* can be assumed to be the Brillouin zone B given by equation (6), i.e. a set of points in 'momentum space'. Assuming the bijection $\psi : \tilde{N} \to B$, given by the formula

$$\psi(l) = \begin{cases} l & \text{for } l \leq N/2 \\ l - N & \text{for } l > N/2 \end{cases} \Bigg\} \, l \in \tilde{N} \tag{A2.7}$$

and defining a one to one mapping of the set $\tilde{N}$ on the symmetric Brillouin zone (symmetric with respect to its centre, $k = 0$), one can write down the regular representation of the dual group C_N^* as

$$\sigma_l = \begin{pmatrix} k \\ \psi((l+k) \bmod N) \end{pmatrix} \qquad l \in \tilde{N} \qquad k \in B \tag{A2.8}$$

i.e. as the counterpart of equation (4) for the 'momentum space', defining the action of the group C_N in the Brilluoin zone B. Both regular representations differ only by labelling of elements of orbits $\tilde{N}$ and B, and of elements of groups C_N and C_N^*; the canonical correspondence between these labellings is given by the bijection ψ and isomorphism λ.

The kernel of the endomorphism $\eta_l \in \text{End } C_N$ is a subgroup $C_\kappa \lhd C_N$ of order

$$\kappa = \text{lcd}(l, N) \tag{A2.9}$$

generated by the complementary divisor $\bar{\kappa}$ in the lattice $K(N)$, i.e.

$$\text{Ker } \eta_l = \{j \in C_N \,|\, lj = N \bmod N\} = \langle \bar{\kappa} \rangle \equiv \{\bar{\kappa}, 2\bar{\kappa}, \ldots, \kappa\bar{\kappa}\} \simeq C_\kappa. \tag{A2.10}$$

Similarly, the image of this endomorphism constitutes the complementary subgroup $C_{\bar{\kappa}} \triangleleft C_N$ generated by κ, i.e.

$$\mathrm{Im}\ \eta_l = \{lj \bmod N \,|\, j \in C_N\} = \langle \kappa \rangle \equiv \{\kappa, 2\kappa, \ldots, \bar{\kappa}\kappa\} \simeq C_{\bar{\kappa}}. \tag{A2.11}$$

Equation (A2.9) defines an equivalence relation in the set $\mathrm{End}\ C_N$, with the corresponding classes

$$(\mathrm{End}\ C_N)_\kappa = \{\eta_l \in \mathrm{End}\ C_N \,|\, \mathrm{lcd}(l, N) = \kappa\} \qquad \kappa \in K(N) \tag{A2.12}$$

labelled by elements κ of the lattice $K(N)$. Each endomorphism in a class $(\mathrm{End}\ C_N)_\kappa$ is characterised by the same kernel and image, given by the groups C_κ and $C_{\bar{\kappa}}$, respectively. It is worth observing that the complementary divisor $\bar{\kappa}$ has a meaning of the order of an endomorphism η_l in the additive group C_N^* of the ring $\mathrm{End}\ C_N$ (so that $\bar{\kappa}\eta_l = \eta_N$, $l \in (\mathrm{End}\ C_N)_\kappa$). In particular, all elements of the class $(\mathrm{End}\ C_N)_1$ are of order N, and their kernels are trivial ($\mathrm{Ker}\ \eta_l = \{N\}$, $1 \in (\mathrm{End}\ C_N)_1$), so that these elements are invertible with respect to multiplication in $\mathrm{End}\ C_N$ (see equation (A2.4)). One thus has

$$(\mathrm{End}\ C_N)_1 = \mathrm{Aut}\ C_N \tag{A2.13}$$

i.e. the class labelled by the minimal divisor $\kappa = 1$ coincides with the group $\mathrm{Aut}\ C_N$, the multiplicative group of the ring $\mathrm{End}\ C_N$. As is known from the theory of numbers, the order of the group $\mathrm{Aut}\ C_N$ is given by the value $\varphi(N)$ of the Euler function $\varphi: Z_+ \to Z_+$ (with Z_+ being the set of all positive integers), i.e.

$$\varphi(N) \equiv |\mathrm{Aut}\ C_N| = \begin{cases} 1 & \text{for } N = 1 \\ N \prod_{p \in \pi(N)} (p-1)/p & \text{for } N > 1. \end{cases} \tag{A2.14}$$

More generally, one has

$$|(\mathrm{End}\ C_N)_\kappa| = \varphi(\bar{\kappa}) \qquad \kappa \in K(N) \tag{A2.15}$$

with the sum rule

$$\sum_{\kappa \in K(N)} \varphi(\bar{\kappa}) = N. \tag{A2.16}$$

It is worth noting that the set $(\mathrm{End}\ C_N)_\kappa \subset C_N^*$ can be looked at as a generalisation of the notion of a conjugacy class in the group C_N. Ordinary conjugacy classes in C_N are orbits of the group $\mathrm{Int}\ C_N = \{\eta_1\}$ of inner automorphisms, consisting only of the unit automorphism η_1, so that they coincide with elements of C_N. The generalisation consists in admitting all automorphisms of the group C_N. $(\mathrm{End}\ C_N)_\kappa$ is thus the orbit generated by $\mathrm{Aut}\ C_N$ from the endomorphism η_κ, i.e.

$$(\mathrm{End}\ C_N)_\kappa = \{\eta_{(l\kappa) \bmod N} \,|\, l \in \tilde{N}, \mathrm{lcd}(l, N) = 1\} \tag{A2.17}$$

and the kernel $\mathrm{Ker}\ \eta_\kappa \simeq C_\kappa$ given by equation (A2.10) is the stability group (the centraliser of the element $\eta_\kappa \in \mathrm{End}\ C_N$ in the group $\mathrm{Aut}\ C_N$), being the same for each of $\varphi(\bar{\kappa})$ elements of this orbit.

Apart from the additive action of the ring $\mathrm{End}\ C_N$ on the one-dimensional crystal $\tilde{N}$ given by equation (4), one can also define the multiplicative action given by equation (A2.2), so that

$$\eta_l = \begin{pmatrix} j \\ lj \bmod N \end{pmatrix} \qquad l \in \tilde{N} \qquad j \in \tilde{N}. \tag{A2.18}$$

Whereas the additive action can be naturally interpreted in terms of translations of the crystal, the multiplicative action cannot be immediately looked at as a generalisation of a rotation of the crystal, because of the kernel Ker η_l given by equation (A2.10). Such an interpretation can be admitted only for the group Aut $C_N \subset$ End C_N, since only then is this kernel trivial. Let us define the action of the set of pairs $(l, \eta_{l'})$, $l \in \tilde{N}$, $l' \in \tilde{N}$, on the crystal $\tilde{N}$ as the composition of actions (4) and (A2.17), i.e.

$$(l, \eta_{l'}) = \begin{pmatrix} j \\ (l + l'j) \bmod N \end{pmatrix} \qquad l \in \tilde{N} \qquad l' \in \tilde{N} \qquad j \in \tilde{N}. \tag{A2.19}$$

The restriction to such pairs $(l, \eta_{l'})$, for which $\eta_{l'} \in$ Aut C_N, yields a group called a holomorph (Hall 1959, Kurosh 1960), i.e.

$$\text{Hol } C_N = C_N \square \text{ Aut } C_N = \{(l, \eta_{l'}) \mid l \in \tilde{N}, \eta_{l'} \in \text{Aut } C_N\} \tag{A2.20}$$

being a semidirect product of the 'passive' group C_N with the 'active' group Aut C_N (C_N being embedded invariantly in Hol C_N). Equation (A2.19) implies the group multiplication for Hol C_N as

$$(l_1, \eta_{l_1'})(l_2, \eta_{l_2'}) = ((l_1 + l_1' l_2) \bmod N, \eta_{(l_1' l_2') \bmod N}). \tag{A2.21}$$

The group Hol C_N thus constitutes a natural generalisation of the notion of a space group for the crystal $\tilde{N}$, with C_N as the translation group and Aut C_N as a group of generalised rotations. In particular, the multiplication law (A2.21) for holomorph takes on the form of the well known Seitz law for a symmorphic space group. Moreover, it is worth noting that the group Aut C_N encloses (for $N > 2$) an invariant subgroup

$$Q = \{\eta_1, \eta_{N-1}\} \lhd \text{Aut } C_N \tag{A2.22}$$

consisting of the unit automorphism η_l and the 'linear inversion'

$$\eta_{N-1} = \begin{pmatrix} j \\ N - j \end{pmatrix} \qquad j \in \tilde{N} \tag{A2.23}$$

consisting of the reflection of all nodes of the chain at the node $j = N$. The subgroup Q is thus an ordinary point symmetry group for a linear chain. All other automorphisms change the cyclic order in $\tilde{N}$ non-trivially, so that they are not isometries of our crystal. The action of an arbitrary automorphism $\eta_l \in$ Aut C_N preserves, however, the decomposition

$$\tilde{N} = \bigcup_{\kappa \in K(N)} \tilde{N}_\kappa \tag{A2.24}$$

where

$$\tilde{N}_\kappa = \{l\kappa \bmod N \mid \eta_l \in \text{Aut } C_N\} \tag{A2.25}$$

is the orbit generated from the node $\kappa \in K(N) \subset \tilde{N}$ by the group Aut C_N. Such orbits are classified by elements of the lattice $K(N)$, in full analogy with equation (A2.12)–(A2.16). An interpretation of a generalised rotation of the crystal $\tilde{N}$ can be admitted only to those permutations $\sigma \in \Sigma_N$ which permute only elements within each subset $\tilde{N}_\kappa$, $\kappa \in K(N)$ in the decomposition (A2.24).

A similar multiplicative action of the ring End C_N can be defined for the Brillouin zone B by putting

$$\zeta(l) = \begin{pmatrix} k \\ \psi(kl \bmod N) \end{pmatrix} \qquad k \in B \qquad l \in \tilde{N}. \tag{A2.26}$$

This action yields the decomposition

$$B = \bigcup_{\kappa \in K(N)} B_\kappa \tag{A2.27}$$

where

$$B_\kappa = \{\psi(l\kappa \bmod N) \,|\, \mathrm{lcd}(l, N) = 1\} \tag{A2.28}$$

is an orbit of the group Aut C_N, in a full analogy with equations (A2.24) and (A2.25). The set B_κ can be interpreted as a generalised star of the wavenumber κ, i.e. the set of wavenumbers generated from $\kappa \in B$ by the group of 'generalised rotations' Aut C_N.

References

Allender D, Bray J W and Bardeen J 1974 *Phys. Rev.* B **9** 119-29
Bak P 1982 *Rep. Prog. Phys.* **45** 587-629
Biedenharn L C and Louck J D 1968 *Commun. Math. Phys.* **8** 89-131
—— 1981 *The Racah-Wigner Algebra in Quantum Theory: Encyclopaedia of Mathematics* vol 9 (Reading, MA: Addison-Wesley)
Bonner J C 1978 *J. Appl. Phys.* **49** 1299-304
Dicke R H 1954 *Phys. Rev.* **93** 99-110
Dyson F J 1956 *Phys. Rev.* **102** 1217-29
Elliott R J, Krumhansl J A and Leath P L 1974 *Rev. Mod. Phys.* **46** 465-543
Foulkes H O 1972 *Proc. Conf. Combinatorial Mathematics* (Oxford: Mathematical Institute) pp 141-54
Fuchs L 1970 *Infinite Abelian Groups* (New York: Academic)
Grätzer G 1978 *General Lattice Theory* (Berlin: Akademie Verlag)
Hall M 1959 *The Theory of Groups* (London: Macmillan)
—— 1967 *Combinatorial Theory* (Waltham, Massachusetts: Blaisdell)
Hasse H 1979 *Number Theory* (Berlin: Akademie Verlag)
Heisenberg W 1928 *Z. Phys.* **49** 619-36
Ising E 1925 *Z. Phys.* **31** 253-8
Kasch F 1977 *Moduln und Ringe* (Stuttgart: Teubner) (*in German*)
Kurosh A G 1960 *Group Theory* (New York: Chelsea)
Lang S 1970 *Algebra* (Reading, MA: Addison-Wesley)
Lulek B and Lulek T 1987 *Acta Phys. Pol.* to be published
Lulek B, Lulek T, Biel J and Chatterjee R 1985a *Can. J. Phys.* **63** 1065-73
Lulek B, Lulek T, Chatterjee R and Biel J 1985b *Can. J. Phys.* **63** 1061-4
Lulek T 1984 *J. Physique* **45** 29-34
Mattis D C 1965 *The Theory of Magnetism* (New York: Harper and Row)
Mermin N O 1979 *Rev. Mod. Phys.* **51** 591-648
Mozrzymas J 1976 *Applications of Group Theory in Physics* (Warsaw: Polish Science Publishers) (*in Polish*) p 35
Narkiewicz W 1977 *Theory of Numbers* (Warsaw: Polish Science Publishers) (*in Polish*)
Newell G F and Montroll E W 1953 *Rev. Mod. Phys.* **25** 353-89
Reiss R F (ed) 1964 *Natural Theory and Modelling* (Stanford, CA: Stanford University Press)
Rybnikov K A 1972 *Introduction to Combinatorial Analysis* (Moscow: Moscow University Press) (*in Russian*)
Satschkov W N 1977 *Combinatorial Methods of Discrete Mathematics* (Moscow: Nauka) (*in Russian*)
Takahashi Y and Shibata S 1976 *J. Stat. Phys.* **14** 49-65
Tsetlin M L 1969 *Investigations in Automata Theory and Modelling of Biological Systems* (Moscow: Nauka) (*in Russian*)
Weyl H 1952 *Symmetry* (Princeton, NJ: Princeton University Press) p 138
Wilson K G and Kogut J 1974 *Phys. Rep.* C **12** 75-200