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Kinematics of the one-dimensional finite Heisenberg magnet with impurities

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Abstract. The kinematics of the one-dimensional finite Heisenberg magnetic ring with impurities is discussed in the light of the general recipe of Weyl. The cyclic group generating the ring, and the group of all its automorphisms, play the roles of the obvious and hidden symmetry, respectively. The hidden symmetry group imposes a property of the distribution of quantum states of a translationally invariant ensemble of magnets over the finite Brillouin zone. Namely, this distribution is constant on each orbit of the action of the hidden symmetry group. It is shown that the above property cannot be broken, neither by any chemical composition of impurities nor by change of their localization. Inhomogeneities of the distribution arise from irregular orbits of the action of the cyclic group on the set of all magnetic configurations of the ensemble. Irregular orbits are indicators of the reference system of 'absolute rest' in the crystal, corresponding to the centre of the Brillouin zone, whereas the case of exclusively regular orbits does not provide such a distinction, so that all quasimomenta enter the theory on the same footing. Size-dependent effects, like rarefied bands, are classified using the arithmetic structure of integers (prime numbers, socles and arithmetic exponents), which is more appropriate than the linear order in the ring of integers.

1. Introduction

We aim to discuss some kinematical properties of the one-dimensional finite Heisenberg model of a magnet with impurities, within the framework of the general recipe of Weyl (1952; cf also references in Florek *et al* 1991). According to the Heisenberg model, the magnet consists of N spins s, localized at nodes of a onedimensional linear ring, and interacting pairwise by an exchange Dirac Hamiltonian. We are interested here in the quantum kinematics rather than dynamics. More specifically, we are looking for the distribution of quantum states of the magnet over the Brillouin zone of the crystal, and for the construction of a space corresponding to each particular quasimomentum.

Hitherto considerations of kinematical properties of the Heisenberg model for the chemically homogeneous magnet (Lulek 1984, Florek and Lulek 1987) and the magnet with a single impurity $s' \neq s$ (Lulek 1988) exhibit two, somehow opposed, tendencies. On the one hand, the finite size of the magnet yields the result that the distribution of quantum states over the Brillouin zone is inhomogeneous, at least for the case of a chemically homogeneous magnet. Details of this inhomogeneity strongly depend on the arithmetic structure of the integer N (Florek and Lulek 1987). On the other hand, breaking of the translational symmetry of the crystal just by a single impurity completely wipes out any inhomogeneity of the distribution of states over the Brillouin zone, for each integer N > 1 (Lulek 1988).

Here, we are going to resolve this apparent puzzle using the general recipe of Weyl (1952) (see also Mozrzymas 1976, 1987, Florek *et al* 1988 and Mucha 1991) and, in particular, our combinatorial approach referred to as the method of irregular orbits (Lulek 1991). It allows us to present transparently and unambiguously kinematical properties of the Heisenberg magnet with impurities. In particular, we discuss the origin of the symmetry property that the distribution of states is constant on the generalized stars in the Brillouin zone, interpreted by Florek and Lulek (1987) as a result of the hidden symmetry Aut C_N of Weyl's recipe. We point out here that this symmetry is even more intrinsically incorporated in basic structural assumptions of the Heisenberg model, since it cannot be broken by any substitution-type impurity, without a change of the structure of a linear ring.

We also clarify the effect of the levelling of inhomogeneity of the considered distribution by impurities. An important point is that this breaking of translational symmetry by an impurity implies that the notion of the Brillouin zone ceases to be applicable. This notion is restored by an appropriate average over an ensemble of magnets with varying localization of impurities. This configuration average is the key reason for the levelling of the size effect in the case of a single impurity. We discuss here the general case of several impurities, and analyse the breaking of translational symmetry for this case.

2. Combinatoric description of the ensemble of magnets with impurities

Let

$$\tilde{N} = \{j \mid j = 1, 2, ..., N\}$$
(1)

be a regular orbit (i.e. an orbit of the left regular representation) of the cyclic group C_N , constituting the set of nodes of a one-dimensional crystal with the Born-Kármán boundary conditions of the period N. Thus C_N is the translation symmetry group of the crystal \tilde{N} . The set

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

of labels of irreps of this group $(\Gamma_k(j) = \exp(2\pi i k j/N))$ where $j \in \tilde{N}$ coincides with the set of all admissible quasimomenta, and will be identified from here with the Brillouin zone of the crystal \tilde{N} .

Let

$$\tilde{l} = \{r \mid r = 1, 2, \dots, l\}$$
(3)

denote the set of labels of all chemically equivalent classes of atoms constituting the crystal \tilde{N} . A distribution of these atoms over the crystal \tilde{N} is given by the mapping $\mu: \tilde{N} \to \tilde{l}$, called the chemical configuration. Each chemical configuration μ defines the decomposition

$$\bar{N} = \bigcup_{r \in I} \mu^{-1}(r) \tag{4}$$

of the crystal \bar{N} into subsets

$$\mu^{-1}(r) = \{ j \in \tilde{N} \mid \mu(j) = r \} \qquad r \in \bar{l}$$
(5)

of nodes with atoms of the type r. The numbers

$$\delta_r = |\mu^{-1}(r)| \qquad r \in \bar{N} \tag{6}$$

of elements of the set $\mu^{-1}(r)$ define the partition

$$\delta = (\delta_1 \dots, \delta_r) \tag{7}$$

of the integer N into l parts, so that

$$\sum_{r \in I} \delta_r = N. \tag{8}$$

Thus the partition δ determines the chemical composition of the crystal. We assume for convenience that $\delta_{r+1} \leq \delta_r \in \tilde{l}$. In particular, δ_1 is the number of atoms of the principal compound, and δ_r for r > 1 is the number of atoms of the *r*th type of impurity.

Magnetic properties of an atom of the rth type are characterized within the Heisenberg model by the spin s_r , and thus by the set

$$\tilde{n}_r = \{i \mid i = 1, 2, \dots, n_r\}$$
 $n_r \equiv 2s_r + 1$ (9)

of projections

$$m_i^r = i - s_r - 1 \qquad i \in \tilde{n}_r \tag{10}$$

of the spin s_r , into a distinguished z-direction in the crystal. An arbitrary magnetic configuration is given by

$$f = |i_1 \dots, i_n\rangle \qquad i_j \in \tilde{n}_r \quad \text{for} \quad j \in \mu^{-1}(r) \subset \tilde{N}.$$
(11)

The set of all magnetic configurations of the crystal \tilde{N} with the chemical configuration μ is the cartesian product

$$\Phi(\mu) = \prod_{r \in I} \times \tilde{n}_r^{\mu^{-1}(r)} \tag{12}$$

of sets of mappings

$$\tilde{n}_r^{\mu^{-1}(r)} = \{ f^r : \mu^{-1}(r) \to \tilde{n}_r \} \qquad r \in \bar{l}$$
(13)

enclosing all magnetic configurations for the rth-type atoms.

The space L of all quantum states of the magnet is the linear unitary space obtained as the linear closure of the set $\Phi(\mu)$ over the field C of complex numbers, which is written as

$$L = \mathbf{k}_C \Phi(\mu) \tag{14}$$

and $\Phi(\mu)$ is an orthonormal basis of L.

An important difficulty with admixtures consists in the observation that neither the set $\Phi(\mu)$, nor the space L, are closed under the action of the translation group C_N (besides the trivial case $\mu = (N, 0, ..., 0)$, corresponding to the chemically homogeneous magnet). Thus the notion of the quasimomentum k loses its meaning within the space L. We avoid this difficulty here in the same way as in our previous paper (Lulek 1988), namely by introducing an ensemble of magnets with some varying chemical configurations, each with the same chemical composition. Formally, an ensemble of magnets is defined as an equivalency class of chemical configurations under the action of a subgroup H of the symmetric group on the set \tilde{N} . In other words, an ensemble is an orbit of the action of the group H on the set

$$\bar{l}^{\bar{N}} = \{\mu : \bar{N} \longrightarrow \bar{l}\}$$
⁽¹⁵⁾

of all chemical configurations. The requirement that the ensemble should be closed under the action of the translation group C_N implies

$$C_N \subseteq H \subseteq \Sigma_N. \tag{16}$$

The choice of an ensemble is thus equivalent to the choice of the subgroup H and of an initial chemical configuration μ . In particular, the choice $H_{\min} = C_N$ preserves the dependence on the internal structure of the chemical configuration μ , i.e. the relative positions of impurities, whereas $H_{\max} = \Sigma_N$ yields only to the dependence on the chemical composition δ . In the following we discuss mainly the case $H = H_{\min} = C_N$. Let

$$\sigma = \begin{pmatrix} j \\ \sigma(j) \end{pmatrix} \in \Sigma_N \qquad j \in \bar{N} \tag{17}$$

be an arbitrary permutation on the set \tilde{N} . Then the ensemble Z of magnets, generated by the subgroup H from the chemical configuration μ , is

$$Z = \{\mu \circ \sigma^{-1} \mid \sigma \in H\}$$
(18)

where $\mu \circ \sigma^{-1} = \mu'$ is the configuration obtained from μ under the permutation σ , i.e.

$$\mu'(j) = \mu(\sigma^{-1}(j)) \qquad j \in \bar{N}. \tag{19}$$

The set of all magnetic configurations, corresponding to the ensemble Z is

$$\Phi_Z = \bigcup_{\mu \in \mathbb{Z}} \prod_{r \in \mathfrak{f}} \tilde{n}_r^{\mu^{-1}(r)}.$$
(20)

Clearly, the number of elements of the ensemble Z is

$$|Z| = \frac{|H|}{|H^{(\mu)}|}$$
(21)

where

$$H^{(\mu)} = \{ \sigma \in H \mid \mu \circ \sigma^{(-1)} = \mu \}$$

$$(22)$$

is the stabilizer of the chemical configuration μ in the subgroup $H \subset \Sigma_N$. The set Φ_Z is already closed under the action $P: \Sigma_N \times \Phi_Z \longrightarrow \Phi_Z$ of the symmetric group Σ_N , defined in a standard way as

$$P(\sigma) = \begin{pmatrix} |i_1, \dots, i_N\rangle \\ |i_{\sigma^{-1}(1)}, \dots, i_{\sigma^{-1}(N)}\rangle \end{pmatrix} \qquad |i_1, \dots, i_N\rangle \in \Phi_Z \qquad \sigma \in \Sigma_N.$$
(23)

Note that the image of the magnetic configuration $|i_1...,i_N\rangle \in \Phi(\mu) \subset \Phi_Z$, corresponding to the chemical configuration $\mu \in Z$, is the magnetic configuration $|i_{\sigma^{-1}(1)},...,i_{\sigma^{-1}(N)}\rangle \in \Phi(\mu \circ \sigma^{-1}) \subset \Phi_Z$, which corresponds to the chemical configuration $\mu \circ \sigma^{-1}$.

Now we are able to define the distribution of states of the ensemble Z over the Brillouin zone B. Let

$$P \downarrow C_N \cong \sum_{k \in B} \oplus m(P \downarrow C_N, \Gamma_k) \Gamma_k$$
(24)

be the decomposition of the restriction $P \downarrow C_N$ of the representation P to the subgroup $C_N \subset \Sigma_N$, acting in the space

$$L_Z = k_C \Phi_Z \tag{25}$$

into irreps of C_N , with multiplicities $m(P \downarrow C_N, \Gamma_k)$. Then the formula

$$\varrho(k) = \frac{m(P \downarrow C_N, \Gamma_k)}{|Z|} \qquad k \in B$$
(26)

defines the distribution $\rho: B \to Q$ of quantum states of the ensemble Z over the Brillouin zone, with Q being the field of all rational numbers.

3. The recipe of Weyl

An adequate framework for the discussion of symmetry breaking is provided by Weyl's recipe (1952), which states that the intrinsic features of a system equipped with a symmetry G, called the obvious symmetry group, emerge from a careful study of the group Aut G of all automorphisms of the group G. The group Aut G is then referred to as the 'hidden' symmetry of the system. In our case, the system under investigation is the ensemble Z of Heisenberg magnets, each magnet endowed with the structure of a regular orbit of the translation group C_N . Chemical and magnetic properties of the ensemble Z are specified by the set Φ_Z of all magnetic configurations for various distributions of component atoms over the crystal \overline{N} . Clearly, an evident candidate for the obvious symmetry is $G = C_N$, the cyclic group of order N.

The group C_N of the obvious symmetry of the model is described in terms of the arithmetic structure of the integer N. Let

$$N = \prod_{p \in \pi(N)} p^{\alpha_{\bullet}(N)}$$
⁽²⁷⁾

be the canonical decomposition of N into prime factors. Here, $\pi(N)$ is the set of all prime divisors of N, known as the socle of N, and $\alpha_p(N), p \in \pi(N)$, are arithmetic exponents of N. We refer hereafter to (27) as the arithmetic structure of N. The lattice K(N) of all subgroups of the translation group C_N coincides with that of all divisors of N

$$K(N) = \left\{ \kappa = \prod_{p \in \pi(N)} p^{\alpha_p(\kappa)} | 0 \leq \alpha_p(\kappa) \leq \alpha_p(N), p \in \pi(N) \right\}$$
(28)

where the partial order is imposed by divisibility, the minimal element is $\kappa_{\min} = 1$, and the maximal $\kappa_{\max} = N$. The structure of the lattice K(N) is transparently presented in a $|\pi(N)|$ -dimensional space spanned by the socle $\pi(N)$. Namely, the lattice K(N) can be looked at as the set of nodes of a finite $|\pi(N)|$ -dimensional crystal, with the socle $\pi(N)$ as the elementary Bravais cell, repeated $\alpha_p(N)$ times in the direction $p \in \pi(N)$. Thus, mutual incommensurability of different prime numbers is reflected geometrically in terms of points in a $|\pi(N)|$ -dimensional space of arithmetically independent variables, i.e. arithmetic exponents $\alpha_p(\kappa), p \in \pi(N)$. The lattice K(N) serves to express in an invariant way most of the essential structures associated with the group C_N , like the lattice of subgroups (i.e. K(N) itself), lattices of epikernels in stratification of actions of C_N on various sets, generalized stars in the Brillouin zone, etc. In particular, each orbit of the cyclic group C_N is uniquely characterized by the stabilizer $C_{\kappa} \triangleleft C_N$ of this orbit, labelled by an element $\kappa \in K(N)$. Clearly, the number of elements of such an orbit is

$$\bar{\kappa} = \frac{N}{\kappa} \qquad \kappa \in K(N)$$
(29)

i.e. the divisor $\tilde{\kappa} \in K(N)$, complementary to κ in the lattice K(N). The case $\kappa = 1$, i.e. $\tilde{\kappa} = N$, corresponds to an orbit of the regular representation, i.e. the free action of the group C_N . Each such orbit consists of N elements, and is referred to hereafter as a regular orbit, whereas each $\kappa > 1$ defines a type of irregular orbit, with $\tilde{\kappa} < N$ elements.

Elementary number theory implies that the hidden symmetry group of Weyl's recipe is

Aut
$$C_N = \left\{ r_r = \begin{pmatrix} j \\ rj \mod N \end{pmatrix}, j \in C_N \mid r \in \tilde{N}, \operatorname{lcd}(r, N) = 1 \right\}$$
 (30)

where lcd (r, N) denotes the largest common divisor of integers r and N. The elements of Aut C_N are automorphisms $\tau_r : C_N \to C_N$, labelled by all those positive integers r < N, which are relatively prime to N. In particular, τ_1 is the unit element of Aut C_N , $\tau_{N-1} \equiv \tau_{-1}$ corresponds to a one-dimensional inversion of the crystal \tilde{N} at the node $j = N \equiv 0 \mod N$, whereas all other elements τ_r can be interpreted as some self-similar, or fractal-like, transformations on \tilde{N} (Lulek *et al* 1991, Kuźma 1991).

Hidden symmetry Aut C_N is displayed, according to the Weyl's recipe, in some intrinsic features of the system. In particular, we consider here kinematical properties, i.e. we are looking for spaces of all accessible states of a stationary motion within the system. We thus expect that the group Aut C_N should be reflected in some

symmetry properties of the distribution ρ of such states over the Brillouin zone B. Indeed, Florek and Lulek (1987) have shown that for the case of a single chemically homogeneous magnet the distribution ρ is constant on each orbit of the action of the hidden symmetry group Aut C_N on the Brillouin zone B. In more detail, the action Ψ : Aut $C_N \times B \to B$, given by

$$\Psi(r) = \begin{pmatrix} k \\ rk \mod N \end{pmatrix} \qquad r \in \operatorname{Aut} C_N \qquad k \in B \tag{31}$$

decomposes the Brillouin zone

$$B = \bigcup_{\kappa \in K(N)} B^{(\kappa)}$$
(32)

into orbits

$$B^{(\kappa)} = \{ r \kappa \mod N \mid r \in \operatorname{Aut} C_N \} \qquad \kappa \in K(N)$$
(33)

(for brevity, we write r instead of τ_r), labelled by elements of the lattice K(N). Each orbit $B^{(\kappa)}$ is referred to as a generalized star of the wavenumber, in accordance with an analogy between the hidden symmetry group Aut C_N and the crystallographic point groups (Florek *et al* 1988). The distribution ρ for the chemically homogeneous magnet is thus constant on each generalized star $B^{(\kappa)}$, i.e.

$$\rho(k) = \text{constant} \quad k \in B^{(\kappa)} \text{ for each } \kappa \in K(N).$$
 (34)

It implies that the hidden symmetry Aut C_N manifests itself in the symmetry of kinematical properties of the magnet.

Florek and Lulek (1987) have expressed the opinion that the property (34) of symmetry of the distribution ρ of quantum states of a Heisenberg magnet in the Brillouin zone *B* can be broken by impurities. In the next section we show that it is not the case, i.e. that this property still holds for an arbitrary composition δ as well as for an arbitrary chemical configuration μ of impurities.

4. The method of irregular orbits and the rarefied Brillouin zones

We proceed to evaluate the distribution ρ for the ensemble Z of magnets, using our method of irregular orbits (Lulek 1991a, b). The method is based on stratification of the set Φ_Z of all magnetic configurations of the ensemble Z under the action $P \downarrow C_N$ of the cyclic group C_N , i.e. on the structure of the set of all orbits of C_N on Φ_Z .

Let $\mathcal{O}_{\kappa} \subset \Phi_{Z}$ be an orbit of the group C_{N} on the set Φ_{Z} with the stabilizer $C_{\kappa}, \kappa \in K(N)$. The key observation is that

$$P \downarrow C_N \mid_{\mathcal{O}_{\kappa}} \cong \sum_{k \in B/\kappa} \oplus \Gamma_k$$
(35)

where the set B/κ is a subset of the Brillouin zone B, given by

$$B/\kappa = \{k \in B \mid \kappa \in K(|k|)\}.$$
(36)

In other words, the restriction of the action $P \downarrow C_N$ to the orbit \mathcal{O}_{κ} or, more accurately, to the linear space

$$L_{\kappa} = k_C \ \mathcal{O}_{\kappa} \tag{37}$$

decomposes into irreps Γ_k of C_N in such a way that each irrep of the set B/κ enters exactly once, whereas all the remaining irreps from the Brillouin zone B do not enter at all. The subset $B/\kappa \subset B$ consists of all multiples of the wavenumber κ , and is referred to as the κ -tuply rarefied Brillouin zone. Each such rarefied Brillouin zone B/κ yields, through the eigenproblem for an appropriate Hamiltonian, a rarefied energy band, i.e. such a band which encloses altogether κ rather than N states. These states are seeded discretely, but uniformly, within the 'full' Brillouin zone $B \equiv B/1$ (Lulek 1984, Florek and Lulek 1987, Lulek 1991a, b).

In this way, the total distribution ρ can be put in a form

$$\varrho(k) = \sum_{\kappa \in K(N)} \varrho_{\kappa}(k) \tag{38}$$

of contributions ρ_{κ} arising from the stratum consisting of all orbits of type κ , i.e.

$$\rho_{\kappa}(k) = \begin{cases} m(P,\kappa)/|Z| & \text{for } k \in B/\kappa \\ 0 & \text{otherwise} \end{cases}$$
(39)

with $m(P,\kappa)$ denoting the number of orbits of C_N with the stabilizer C_{κ} on Φ_Z . The latter can be readily evaluated by combinatorial methods (Burnside lemma) as

$$m(P,\kappa) = \sum_{\kappa' \in K(N)} B_{\kappa\kappa'}(C_N) |\Phi_Z^{(\kappa')}|$$
(40)

where

$$|\Phi_Z^{(\kappa')}| = |\{f \in \Phi_Z | f \circ \sigma^{-1} = f, \sigma \in C_{\kappa'}\}|$$
(41)

is the number of fixed elements of the set Φ_Z under the action $P \downarrow C_{\kappa'}$ of the subgroup $C_{\kappa'} \triangleleft C_{\kappa}$, and $B_{\kappa\kappa'}(C_N)$, $\kappa, \kappa' \in K(N)$, are elements of the Burnside matrix for the group C_N (Kerber *et al* 1991). The latter is given by

$$B_{\kappa\kappa'}(C_N) = \begin{cases} \bar{\kappa}\mu(\kappa'/\kappa) & \text{ for } \kappa \in K(\kappa') \\ 0 & \text{ otherwise} \end{cases}$$
(42)

and μ is the Möbius function of number theory, given by

$$\mu(N) = \begin{cases} 1 & \text{for } N = 1\\ (-1)^{|\pi(N)|} & \text{for } \alpha_p(N) = 1, \ p \in \pi(N) \\ 0 & \text{otherwise} \end{cases}$$
(43)

(cf equation (27)). In particular, the case of a chemically homogeneous magnet yields (Florek and Lulek 1987)

$$\varrho_{\kappa}(k) = \frac{1}{N} n^{\hat{\kappa}} \varphi(\kappa) \mu(\kappa') / \varphi(\kappa') \qquad k \in B^{(\kappa_{\bullet})}$$
(44)

where $\kappa' = \operatorname{lcd}(\bar{\kappa}\kappa_{o}, N)$, and φ is the Euler function of number theory, given by

$$\varphi(N) \equiv |\operatorname{Aut} C_N| = \prod_{p \in \pi(N)} p^{\alpha_p(N) - 1}(p-1).$$
(45)

In this way, the homogeneous part of the distribution ρ arises from the full bands, corresponding to regular orbits ($\kappa = 1$) of action of the translation group C_N on the set Φ_Z of all magnetic configurations of the ensemble Z of magnets. In other words, a regular orbit contributes exactly one quantum state of the ensemble Z for each wavenumber k of the Brillouin zone B. On the other hand, inhomogeneity of this distribution is related to rarefied bands, which correspond to irregular orbits, i.e. orbits with the non-trivial stabilizer $C_{\kappa}, \kappa > 1$. An irregular orbit of the type κ spreads over the rarefied Brillouin zone $B/\kappa \subset B$, i.e. contributes one state for each multiple of κ in B, and yields a vacancy for any other wavenumber $k \in (B \setminus (B/\kappa))$. It results in inhomogeneity of the total distribution ρ .

We are thus left with all irregular orbits of C_N on Φ_Z . These, and only these, orbits give rise to inhomogeneities of the distribution ϱ . Such an orbit is characterized by its stabilizer, which is a non-trivial subgroup $C_{\kappa} \triangleleft C_N, \kappa > 1$. Clearly, the orbit itself exhibits the translational symmetry, given by its stabilizer C_{κ} . In other words, the translational symmetry C_N of the system is not broken at this orbit totally (as in the case of an arbitrary regular orbit), but only partially. The orbit itself can be looked at as a new periodic structure, with the Born-Kármán period κ instead of N, and the new elementary Bravais cell enclosing $\bar{\kappa}$ nodes. Thus such an irregular orbit corresponds to a phase with broken translational symmetry, resulting from a Peierls-like phase transition with a $\bar{\kappa}$ -tuply enlarged elementary cell of the prototypic phase (Peierls 1955; cf Kuźma *et al* 1989, 1991). The breaking of translational symmetry results either from impurities, i.e. chemical configurations, or from the shape of magnetic configurations, or from a combination of both.

In the case of a chemically homogeneous magnet, |Z| = 1, the breaking of translational symmetry results exclusively from the shape of magnetic configurations within an orbit. In the case of a regular orbit the elementary Bravais cell of a magnetic configuration coincides with the whole crystal, and yields an homogeneous contribution to the distribution ρ . Inhomogeneity of ρ emerges from all those magnetic configurations which exhibit an elementary Bravais cell of the size $\bar{\kappa} < N$. It is discussed in detail elsewhere (Lulek 1991a).

The case of a single impurity, $\delta = (N - 1, 1)$, $H = C_N$, and thus |Z| = N, yields that Φ_Z consists exclusively of regular orbits of the group C_N . It results from the observation that all elements of an orbit of C_N in Φ_Z differ mutually by the position of the impurity (cf equation (23)). The distribution ρ is given therefore by the simple formula

$$\varrho(k) = (2s+1)^{N-1}(2s'+1)/N \qquad k \in B \tag{46}$$

and is homogeneous in the Brillouin zone B (Lulek 1988). Thus the picture of orbits displays unambiguously the somehow surprising result of a complete levelling of inhomogeneity of ρ by a single impurity.

In the general case, i.e. for an arbitrary chemical composition ρ , the stabilizer of a chemical configuration μ in the symmetric group Σ_N is the Young subgroup

$$\Sigma(\mu) = \prod_{r \in I} \times \Sigma_{\mu(r)}$$
(47)

i.e. the outer direct product of symmetric groups, each acting on the subset of chemically equivalent nodes. Thus the chemical configuration μ can yield an irregular orbit of magnetic configurations only in the case when the intersection

$$C_N \bigcap \Sigma(\mu) = C_\kappa \tag{48}$$

is non-trivial, i.e. $\kappa > 1$. In particular, it is clear that this condition cannot be satisfied for a single impurity, i.e. for $\delta = (N - 1, 1)$, since

$$(\Sigma_{N-1} \times \Sigma_1) \bigcap C_N = C_1. \tag{49}$$

In the case of two admixtures, i.e. $\delta = (N-2,2)$, the condition (48) can be satisfied only for even N and antipodal chemical configurations, i.e. when admixed ions occupy mutually antipodal positions in the chain. In this case

$$C_N \bigcap \left(\Sigma_{N-2} \times \Sigma_2 \right) = \begin{cases} C_2 \equiv \Sigma_2 & \text{for antipodal chemical configurations} \\ C_1 & \text{otherwise.} \end{cases}$$
(50)

In general, irregular orbits emerge only in cases of a symmetric distribution of impurities in the chain, so that there remains a non-trivial translational symmetry.

We proceed to discuss the symmetry property (34) of the distribution ρ . With this aim, we observe that

$$B/\kappa = \bigcup_{\{\kappa' \in K(N) | \kappa' / \kappa \in K(\bar{\kappa})\}} B^{(\kappa')}$$
(51)

which implies that each rarefied Brillouin zone B/κ is a union of some complete generalized stars of B. It also follows that the distribution $\rho: B \to Q$ for the ensemble Z of magnets is constant on each generalized star $B^{(\kappa)} \subset B, \kappa \in K(N)$, for an arbitrary chemical composition and spatial distribution of atoms.

We have thus shown that the symmetry property (34) is deeply associated with the orbit structure of the space L_Z of all quantum states of the ensemble Z, and cannot be broken by any change in chemical structure. The breaking of this symmetry property can be done in a way that violates some model assumptions for the Heisenberg magnet. It can be performed by, for example, some constraints for admissible quantum states, such that the resultant space $L'_Z \subset L_Z$ cannot span over orbits of the translation group C_N .

5. An example

The existence of rarefied bands, as well as their selective levelling by impurities, can be demonstrated on a simple, but representative enough, example of N = 12, the chemical composition $\delta = (8,4), s = 1/2$ and s' = 1. The set of

$$\begin{pmatrix} 12\\4 \end{pmatrix} = 495 \tag{52}$$

different chemical configurations corresponding to this composition forms an orbit of the symmetric group Σ_{12} , with the Young subgroup $\Sigma(8, 4)$ as the stabilizer. The

associated transitive representation $\Re^{\Sigma_{12}:\Sigma(8,4)}$ decomposes under the subduction of Σ_{12} to C_{12} as

$$\Re^{\Sigma_{12}:\Sigma(8,4)} \downarrow C_{12} = 40 \Re^{12:1} + 2 \Re^{12:2} + \Re^{12:4}$$
(53)

into transitive representations $\Re^{N:\kappa}$ of the group $C_N = C_{12}$ with the stabilizer C_{κ} , $\kappa \in K(12)$. The lattice K(12) is presented in figure 1. Assuming $H = C_{12}$ as the group that defines the configuration average, we distinguish three kinds $Z_i, i = 1, 2, 3$, of ensembles of magnets. The ensemble Z_1 corresponds to regular orbits ($\kappa = 1, |Z_1| = 12$), Z_2 to (chemically) irregular orbits of the type $\kappa = 2$ ($|Z_2| = 6$) and Z_3 to $\kappa = 4$ ($|Z_3| = 3$). Thus the ensemble Z_1 exhibits completely broken translational symmetry, whereas the other two carry some residual' invariance, described by their stabilizers $C_{\kappa} \triangleleft C_{12}$. The size $N' = \tilde{\kappa}$ of the elementary Bravais cell is N' = 12, 6, and 3 for the ensemble $Z_1, Z_2, \text{ and } Z_3$, respectively. The sequences

and

h h i

with h and i denoting the host and impurity atom, respectively, serve as examples of chemical configurations of the Bravais cell for the ensemble Z_2 and Z_3 , respectively.



Figure 1. The lattice K(12). Arrows indicate the partial order. Observe that this partial order is not consistent with the linear order (1, 2, 3, 4, 6, 12).

The set $\Phi(\mu)$ for a chemical configuration μ belonging to any kind of ensemble encloses $|\Phi(\mu)| = 2^8 \times 3^4 = 20736$ magnetic configurations. This set is not closed under the action $P \downarrow C_N$ of the translation group C_N . The corresponding closed sets Φ_Z contain $|\Phi_Z| = 248832$, 124416 and 62 208 elements for the ensemble $Z = Z_1, Z_2$ and Z_3 , respectively. The number $m(\Phi, \kappa)$ of orbits of type $\kappa \in K(N)$ can be evaluated using (40) with the Burnside matrix

$$B(C_{12}) = \begin{pmatrix} \frac{1}{12} & -\frac{1}{12} & -\frac{1}{12} & \cdot & \frac{1}{12} & \cdot \\ & \frac{1}{6} & \cdot & -\frac{1}{6} & -\frac{1}{6} & \frac{1}{6} \\ & & \frac{1}{4} & \cdot & -\frac{1}{4} & \cdot \\ & & & \frac{1}{3} & \cdot & -\frac{1}{3} \\ & & & & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$$
(54)

where rows and columns are labelled in the sequence (1, 2, 3, 4, 6, 12) of elements of K(12) imposed by the linear order of the ring Z (inconsistent with the partial

order shown in figure 1), and dots and empty places denote zeros. The number $|\Phi_Z^{(\kappa')}|$ of fixed points under the action $P \downarrow C_{\kappa'}$ of the subgroup $C_{\kappa'} \triangleleft C_{\kappa} \triangleleft C_{12}$ is determined combinatorically by the size $\bar{\kappa}'$ of the corresponding period. In more detail, if κ' divides both parts, δ_1 and δ_2 of the partition $\delta = (8, 4)$ (thus, if $\kappa' = 1, 2$, or 4), then $|\Phi_Z^{\kappa'}|$ is equal to |Z| times the number of magnetic configurations constructed on the elementary cell of the size $\bar{\kappa}' = N/\kappa'$, with the chemical composition $\delta' = (\delta_1/\kappa, \delta_2/\kappa)$, and otherwise is zero. The resulting values of the number $m(P, \kappa)$ of orbits of type κ for ensembles Z_1, Z_2 and Z_3 are listed in table 1.

Table 1. Numbers of orbits of the type κ in the set Φ_Z of all magnetic configurations of an ensemble Z ($N = 12, \delta = (8, 4), s = 1/2, s' = 1$).

Ensemble	$\kappa = 1$	$\kappa = 2$	$\kappa = 4$
$\overline{Z_1}$	20736	0	0
Z_2	10 296	144	0
$\overline{Z_3}$	5 148	66	12

We observe that most of the orbits are regular ($\kappa = 1$, the first column of table 1), and there are also orbits with the stabilizer C_2 and the elementary magnetic cell consisting of six nodes ($\kappa = 2$), and those with the stabilizer C_4 and the cell consisting of three nodes. Decomposition (32) of the Brillouin zone B into generalized stars has the form

$$B \equiv B/1 = \{12\} \cup \{\pm 1, \pm 5\} \cup \{\pm 2\} \cup \{\pm 3\} \cup \{\pm 4\} \cup \{6\}$$
(55)

and the relevant rarefied Brillouin zones are

$$B/2 = \{12\} \cup \{\pm 2\} \cup \{\pm 4\} \cup \{6\}$$
(56)

$$B/4 = \{12\} \cup \{\pm 4\}. \tag{57}$$

The corresponding distribution ρ , together with the structure of rarefied Brillouin zones and generalized stars, is listed in table 2. The first row for each ensemble Z corresponds to the homogeneous component of ρ , arising from the 'full' Brillouin zone $B/1 \equiv B$, i.e. from regular orbits of C_{12} on Φ_Z , next rows indicate contributions from rarefied Brillouin zones B/κ emerging from irregular orbits, and the last row is the resultant distribution. The ensemble Z_1 exhibits the homogeneous distribution, Z_2 involves an inhomogeneity related to doubly rarefied Brillouin zone.

6. Impurities and rarefied bands

The translation group C_N of the linear chain \bar{N} yields the notion of a quasimomentum k as an irreducible representation, and the Brillouin zone enters as the set of all quasimomenta. In the case of impurities, these notions are abandoned for a single magnet by the breaking of its translational symmetry. They are restored in our approach by use of the average over all translationally equivalent chemical

Ensemble	Rarefied Brillouin zone	Generalized star						
		{12}	{±1,±5}	{±2}	{±3}	{±4}	{6}	
$\overline{Z_1}$	$B \equiv B/1$	1728	1728	1728	1728	1728	1728	
	$B \equiv B/1$	1716	1716	1716	1716	1716	1716	
Z ₂	B/2	24		24		24	24	
	Total	1740	1716	1740	1716	1740	1740	
	$B \equiv B/1$	1716	1716	1716	1716	1716	1716	
Z ₃	B/2	22		22		22	22	
	B/4	4	_	_		4		
	Total	1742	1716	1738	1716	1742	1716	

Table 2. Distribution of quantum states of an ensemble Z of magnets over the Brillouin zone for N = 12, $\delta = (8, 4)$, s = 1/2, s' = 1, with contributions from relevant rarefied Brillouin zones.

configurations. We have examined the distribution ρ of quantum states of the system over the Brillouin zone B.

The distribution ρ is transparently determined by the structure of orbits of the action of the translation group C_N on the set Φ_Z of all magnetic configurations of the ensemble Z of magnets entering the configurational average. The key observation is that an orbit with the stabilizer $C_{\kappa} \triangleleft C_N$ yields the κ -tuply rarefied Brillouin zone B/κ , and thus a single, κ -tuply rarefied band. In this way, the distribution ρ becomes inhomogeneous, depending on the overlap of various rarefied Brillouin zones $B(\kappa), \kappa \in K(N)$. Details of this inhomogeneity are thus described in terms of the lattice K(N) of divisors of N, and depend on the spatial distribution of impurities within the ensemble Z.

In order to present this dependence, assume hypothetically that one is able to prepare a linear magnetic chain, as well as appropriate ensembles of such chains, with the following four properties: (i) each chain consists of exactly N nodes; (ii) each node takes on one of the two values of spin, either s or s' (with respectively 2s + 1 or 2s' + 1 projections); (iii) one can control externally the value of spin at each node, so that it is possible to realize an arbitrary chemical configuration in the crystal \bar{N} ; and (iv) it is possible to determine the structure of energy bands of the system and, in particular, the number of full and rarefied bands of appropriate ensembles. Then our considerations yield the following predictions concerning existence of rarefied bands. (a) A characteristic feature of the chemically homogeneous magnet is the existence of all types of rarefied bands, predicted by the lattice K(N). Full bands ($\kappa = 1$) emerge from all those magnetic configurations that exhibit fully broken translational symmetry, whereas κ -tuply rarefied bands are associated with such magnetic configurations that possesses the magnetic Bravais cell of size $\bar{\kappa} = N/\kappa, \kappa \in K(N)$. (b) When the magnet with impurities with spin s' > s exhibits a residual translational symmetry $C_s \triangleleft C_N$ of chemical configuration, then firstly, all those rarefied bands of the type κ' , for which

$$\kappa' \in \bar{\kappa} K(\kappa) \subset K(N) \tag{58}$$

holds, are selectively enhanced in comparison to the homogeneous case, i.e. $\rho_Z(\kappa') > \rho_h(\kappa')$ with Z and h denoting respectively the ensemble with impurities and the homogeneous magnet, and secondly the remaining rarefied bands, for which $\kappa' \in K(N) \setminus \bar{\kappa} K(\kappa)$, are completely wiped out. In particular, the case $\kappa = 1$ with completely broken translational symmetry yields an exactly homogeneous distribution ρ .

We thus arrive at the general conclusion that the existence of rarefied bands for an ensemble of magnets with impurities is intimately related to the residual translational symmetry. A complete chemical disorder wipes out any rarefied bands, whereas a residual symmetry C_{κ} provides only those bands which are classified by the corresponding lattice $K(\kappa)(\bar{\kappa}K(\kappa))$ being a sublattice of K (N)).

7. Weyl's recipe and kinematical relativity

Weyl's recipe can be looked at as a relativity postulate for any physical system or mathematical model with a general meaning that intrinsic features of the object under investigation should not depend upon any accidental details like labelling of elements of the system, reference frames, and so on (Mozrzymas 1976, 1987). We discuss it here with the specific meaning of kinematical relativity. Quantum states of the Heisenberg magnet with a definite value of quasimomentum k are analogues of free motion of a body in classical mechanics. It is the essence of Newton's First Law that all states of free motion without external fields are mutually equivalent, and can be related to appropriate inertial systems. The relativity postulate imposes the condition that there is no system of 'absolute rest'. In the case of a Heisenberg magnet we do have the analogue of absolute rest, which is the centre k = 0 of the Brillouin zone B, or equivalently, the generalized star $B^{(N)}$. Distinction of this point within the Brillouin zone B in the kinematical aspect manifests itself in the fact that

$$\varrho(0) \ge \varrho(k) \qquad |k| > 0 \tag{59}$$

i.e. that $\rho(0)$ is always the maximal value of the distribution ρ . It is clear from the observation that the generalized star $B^{(N)}$ belongs to each rarefied Brillouin zone

$$B^{(N)} \in B/\kappa \qquad \kappa \in K(N).$$
 (60)

In general, kinematically distinguished points of the Brillouin zone B constitute generalized stars $B^{(\kappa)}$, $\kappa \in K(N)$. Namely, the distribution ρ is constant on each generalized star $B^{(\kappa)}$ for an arbitrary chemical configuration of impurities. This feature can be broken only by some model assumptions which destroy the orbit structure of the space of quantum states of the system.

The case $\kappa = 1$ corresponds to the general position in the Brillouin zone, and is related to the minimal value of the distribution ρ , i.e.

$$\varrho(1) \leq \varrho(k) \qquad k \in B^{(\kappa)} \qquad \kappa > 1.$$
(61)

In this context, it is important to point out the role of irregular orbits $\mathcal{O}_{\kappa}, \kappa > 1$, in the set Φ_Z of magnetic configurations of the ensemble Z. These orbits alone realize the distinction between various generalized stars in the Brillouin zone. This distinction is reflected in the partial order of the lattice K(N), an implicit manifestation of the hidden symmetry Aut C_N of Weyl's recipe. Choosing an appropriate residual symmetry C_{κ} of the chemical configuration, one can enhance selectively various kinds of inhomogeneities of the distribution ϱ . Any non-trivial translational symmetry $C_{\kappa}, \kappa > 1$, results in a kinematic distinction of states of 'absolute rest', i.e. states corresponding to the centre $B^{(N)}$, whereas the case $\kappa = 1$ yields the lack of such a distinction. Thus an ensemble Z with totally broken translational symmetry is an analogy of Galilean invariance in the discrete Brillouin zone.

8. Effects of finite size and arithmetic properties of N

We have discussed hitherto kinematical properties of a magnet, or an ensemble of magnets, with a fixed number N of all nodes. N defines the size of a one-dimensional crystal N. An evident result, emerging unambiguously from this and previous papers (Lulek 1984, Florek and Lulek 1987, Lulek 1988, 1989a, b) is the strong dependence of characteristics of a finite crystal on the arithmetic structure of N. This dependence manifests itself, in particular, in the prominent role of the lattice K(N) of all divisors of N. This lattice proves to be an adequate tool in a complete description of such physical characteristics as the classification of Peierls-like phase transitions related to all possible ways of breaking translational symmetry (Kuźma *et al* 1989, 1991), or labelling the types of rarefied bands.

At first sight, this feature seems to be inconsistent with a common opinion that intrinsic properties of a sufficiently large system should not depend on the arithmetic structure of N. However, at this point we have to distinguish between two things: the bulk properties of crystals, which do not depend on N, and the effects of a finite size of a particular crystal, which are N-dependent. Thus full energy bands are present in each crystal and can be—in general—attributed to bulk properties, whereas rarefied bands are typical characteristics of a finite crystal.

One can put the question of a physical classification of size effects in the set of all magnets \overline{N} . Contrary to some temptations based on a naive intuition, the 'natural' linear order in the ring Z of integers is not a proper basis for such an aim. The main reason is that a change of N according to the linear order yields a highly intricate behaviour of kinematical properties of magnets, involving rapid variations of appropriate lattices K(N), their socles $\pi(N)$, as well as the corresponding arithmetic exponents. On the other hand, a change of N in accordance with the partial order suggested by the arithmetic structure of integers yields a much more straightforward description.

Let us first consider the set

$$C(p) = \{\bar{N} | N = p^{\alpha}, \alpha = 1, 2, \ldots\}$$
(62)

of all crystals \tilde{N} , where N is a power of the single prime number p. The lattice

$$K(p^{\alpha}) = \{ \kappa = p^{\alpha'} | 0 \leqslant \alpha' \leqslant \alpha \}$$
(63)

is characterized now by the linear order of arithmetic exponents, and yields

$$K(p^{\alpha-1}) \subset K(p^{\alpha}) \tag{64}$$

i.e. each lattice $K(p^{\alpha})$ covers all preceding lattices with $\alpha' < \alpha$. The minimal quantum of quasimomentum for $N = p^{\alpha}$ is $2\pi/p^{\alpha}$, and an increase of the arithmetic exponent $\alpha \equiv \alpha_p(N)$ yields a denser distribution of the discrete Brillouin zone B in the segment

$$B_c = (-\pi, \pi] \tag{65}$$

with the factor 1/p. Crystals within each set C(p) have simple kinematical properties, determined by a single arithmetic exponent α . For example, the number of $p^{\alpha'}$ -tuply rarefied bands of the homogeneous crystal for $N = p^{\alpha}$ is

$$m(P, p^{\alpha'}) = p^{\alpha' - \alpha} n^{p^{\alpha' - 1}} (n^p - 1) \qquad \alpha' \leq \alpha.$$
(66)

Now assume that π is a set of prime integers, $|\pi| > 1$, and consider the set

$$C(\pi) = \{ \tilde{N} | N \in Z_+, \pi(N) = \pi \}$$
(67)

of all crystals with the same socle π . Appropriate lattices K(N) already have non-trivial partial orders, since arithmetic exponents $\alpha_p(N)$ and $\alpha_{p'}(N), p \neq p'$, are no longer comparable. It is reflected in the observation that quanta of quasimomentum, corresponding to different prime numbers, are incommensurate. Kinematical properties of crystals of the set $C(\pi)$ display a regularity consistent with the partial order imposed by the multidimensional socle π , but are not necessarily smooth with respect to the linear order imposed by the ring Z of integers.

We observe therefore that N can increase in two essentially different ways: (i) by an increase of the socle π , i.e. by the addition of some new prime numbers p, or (ii) by an increase of arithmetic exponents α_p . Case (ii) yields a smooth variation of kinematical properties of the crystal, whereas case (i) introduces qualitatively new features. The situation is demonstrated in figure 2 for the three-dimensional socle $\pi = \{2, 3, 5\}$. All elements of the lattice K(360) presented in this figure (and, in particular, the clock dial plate of section 5) correspond to a possible broken Peierls-like phase of the crystal with N = 360 states.



Figure 2. The lattice K(360) presents a three-dimensional parallelepiped, built on the socle $\pi = \{2, 3, 5\}$, as the elementary Bravais cell, with arrows on edges indicating the partial order. An increase of N by multiplication can be done by a combination of two operations. (i) Addition of further primes to the socle π , which results in enlarging of dimension $|\pi(N)|$ of the lattice K(N). (ii) Increase of arithmetic exponents $\alpha_p(N), p \in \pi(N)$, which yields an appropriate extension of the parallelepiped K(N). The operation (i) is responsible for qualitative changes of kinematical properties of magnets, inconsistent with the linear order of integers, whereas the operation (ii) yields only smooth variations of them.

It is worthwhile to observe that the limit $N \to \infty$ (taken according to the linear order in Z) excludes all fractal symmetries of finite crystals. Within the recipe of Weyl, we have

$$\operatorname{Aut} Z = Z_2 = \{\tau_1, \tau_{-1}\}$$
(68)

whereas each (large enough) N yields

$$|\operatorname{Aut}C_N| = \varphi(N) \ge 2 \qquad N > 2.$$
 (69)

It can be interpreted that the group Aut Z of the hidden symmetry of the infinite chain is the subgroup of all hidden symmetry groups Aut C_N , N > 2, and each of them encloses the one-dimensional inversion τ_{-1} —the only non-trivial common element of all these groups.

Crystals \tilde{N} with various arithmetic properties distinguish different subsets $(\pi/N)B \subset B_{\mathbb{C}}$ of the continuous Brillouin zone $B_{\mathbb{C}}$. In principle, standard calculations of spectral density of states involving integration over the continuous Brillouin zone $B_{\mathbb{C}}$ should be replaced by summation over the corresponding discrete Brillouin zone B, using the appropriate inversion formulae of Möbius instead of differential calculus. Weyl's recipe suggests that the natural subsets of the discrete Brillouin zone B in substituting differentials by differences are generalized stars $B^{(\kappa)}, \kappa \in K(N)$. They are entirely sufficient with respect to kinematical properties (even in the case of impurities), and require some further division into smaller subsets in analysing the dynamics.

Rarefied bands are, in general, not too important in statistical physics since the limit $N \to \infty$ implies that the ratio of these bands to the total number of quantum states tends exponentially to zero (cf equation (44)). These bands can, however, be dynamically important in two aspects. First, they should be taken into account for sufficiently small N, e.g. in macromolecules or in physics on the mesoscopic scale. In the extremely small case, N = 2, i.e. for the ground spin states of the hydrogen molecule, triplet states S = 1 correspond to the centre k = 0 of the discrete Brillouin zone $B = \{0, 1\}$, whereas the singlet state S = 0 corresponds to the boundary k = 1. Thus $2^2 = 4$ states of the spin s = 1/2 on N = 2 nodes can be arranged into three bands: one full band for M = 0, and two doubly rarefied (it means here single states) for $M = \pm 1$. Secondly, the role of rarefied bands becomes important in such cases when they have a relatively low energy. In these situations they also become meaningful on the macroscopic scale, e.g. in Peierls phase transitions (Kuźma *et al* 1989, 1991), since they are immediately related to the shape of the elementary Bravais cell.

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