PUBL. I.R.M.A. STRASBOURG, 1991, 476/S-26
ACTES 26^e SÉMINAIRE LOTHARINGIEN, P. 55-62

Impurities in the Heisenberg magnet and the general recipe of Weyl

B.Lulek

Abstract

The general recipe of Weyl is applied to the Heisenberg model of a one-dimensional magnetic chain with impurities. It is found that impurities break the obvious translational symmetry, but preserve the hidden one. Rarefied bands emerge from irregular orbits of action of the translation group.

1 Introduction

We examine here an application of the general recipe of Weyl [1,2] to the Heisenberg model of a magnet [3,4]. It has been shown that the hidden symmetry group of Weyl's recipe yields some symmetries of the distribution of quantum states of a magnet within the Brillouin zone [3], and that these symmetries can be described in terms of rarefied bands [3,4]. These results, obtained for a crystal with the perfect translational symmetry, can be discussed again for crystals with broken periodicity, caused by impurities. We have discussed already the case of a single impurity [5], and found an apparently puzzling result that breaking of translational symmetry increases, rather than decreases, the symmetry of this distribution. Here we proceed to discuss a more general case of some impurities in the light of the recipe of Weyl. In particular, we aim to point out that breaking of translational symmetry is equivalent to decreasing of the obvious symmetry group, which does not automatically imply lowering of the hidden symmetry [6].

2 The recipe of Weyl

Let us assume that we have a system with some *obvious symmetry*, described by a group G. A good example is a system that constitutes a regular orbit of this group, so elements of the system can be labelled by $g \in G$. The recipe of Weyl states that then all intrinsic features of the system are derivable from the group Aut G, the group of all automorphisms of G. This group, Aut G, is called the *hidden symmetry* group of the system.

3 The homogeneous magnet

Let

$$X = \{j \mid j = 1, 2, \ldots, n\} \tag{1}$$

be the set of all n nodes of a crystal. Within the Heisenberg model of a magnet, one assumes that each node $j \in X$ is occupied by a spin s. Let

$$Y = \{i \mid i = 1, 2, \ldots, m\} \tag{2}$$

be the set of labels of projections $-s, -s+1, \ldots, +s$ of the spin s, so that $m = 2s+1$. Any mapping $f : X \to Y$ is called a magnetic configuration. It can be displayed in a form

$$f = |i_1, \ldots, i_n\rangle, \quad i_j \in Y, \; j \in X. \tag{3}$$

The set of all magnetic configurations is

$$Y^X = \{f : X \to Y\}. \tag{4}$$

We assume that n nodes of our crystal are arranged into a one-dimensional finite chain, or, more precisely, that the set X constitutes a regular orbit of the cyclic group

$$G = C_n, \tag{5}$$

the translational symmetry group of the magnet. We take C_n as the obvious symmetry group of Weyl's recipe.
We denote by

$$B = \{k = 0, \pm 1, \pm 2, \ldots, \begin{cases} \pm(n/2-1), n/2 & \text{for } n \text{ even} \\ \pm(n-1)/2 & \text{for } n \text{ odd} \end{cases}\} \tag{6}$$

the set of labels of all irreducible representations of the group C_n over the field $\mathbb{C}$ of complex numbers. This set is referred to as *the Brillouin zone* in condensed matter physics.
We proceed to define the distribution of quantum states of the magnet over the Brillouin zone B. Let $P : S_n \times Y^X \to Y^X$ be the action of the symmetric group S_n on the set Y^X of all magnetic configurations. This action is defined by the formula

$$P(\sigma) = \begin{pmatrix} f \\ f \circ \sigma^{-1} \end{pmatrix}, \quad f \in Y^X, \quad \sigma \in S_n. \tag{7}$$

Let, moreover,

$$L = \mathrm{lc}_{\mathbb{C}} Y^X \tag{8}$$

be the linear closure over the field $\mathbb{C}$, spanned on the set Y^X, with the unitary structure imposed by requirement that Y^X is an orthonormal basis in L. We denote the action of the group S_n in the linear unitary space L by the same letter P. Under the embedding $C_n \subset S_n$ this action subduces to

$$P \downarrow C_n \cong \bigoplus_{k \in B} \rho(k)\Gamma_k, \tag{9}$$

where Γ_k is an irreducible representation of C_n. The decomposition (9) defines the mapping $\rho : B \to \mathbb{Z}$ of B into the ring $\mathbb{Z}$ of integers, called the *distribution of quantum states* of the magnet *over the Brillouin zone* B. This distribution can be evaluated as [4,7,8]

$$\rho(k) = \frac{1}{n} \sum_{\kappa \in K(n)} n^{\kappa} \frac{\varphi(\bar{\kappa})}{\varphi(\bar{\kappa'})} \mu(\bar{\kappa'}), \tag{10}$$

where

$$K(n) = \{\kappa \in X \mid \text{lcd}(n, \kappa) = \kappa\} \tag{11}$$

is the lattice of all divisors of the integer n,

$$\bar{\kappa} = n/\kappa \tag{12}$$

is the divisor complementary to κ in the lattice $K(n)$, $\varphi : K(n) \to \mathbb{Z}$ and $\mu : K(n) \to \mathbb{Z}$ is the Euler and Möbius function, respectively, and

$$\kappa' = \text{lcd}(\kappa\kappa_0, n), \tag{13}$$

$$\kappa_0 = \text{lcd}(|k|, n), \tag{14}$$

with lcd denoting the largest common divisor.
The symmetry of the distribution ρ is described by

$$\text{Aut}\, C_n = \{r \in X \mid \text{lcd}(r, n) = 1\}, \tag{15}$$

the hidden symmetry group of the recipe of Weyl [3,4,9]. Let $\Psi : \text{Aut}\, C_n \times B \to B$ be the action of $\text{Aut}\, C_n$ on the Brillouin zone B, defined by the formula

$$\Psi(r) = \begin{pmatrix} k \\ rk \bmod n \end{pmatrix}, \quad k \in B, \ \text{lcd}(r, n) = 1. \tag{16}$$

The action Ψ yields orbits

$$B^{(\kappa)} = \{k \in B \mid \text{lcd}(k, \kappa) = \kappa\}, \quad \kappa \in K(n), \tag{17}$$

called *generalized stars*. Thus the Brillouin zone decomposes into disjoint generalized stars as

$$B = \bigcup_{\kappa \in K(n)} B^{(\kappa)}. \tag{18}$$

Theory of condensed matter bases heavily on the notion of a band. A *full band* corresponds to a such distribution of system states over the Brillouin zone B, in which each

quasimomentum $k \in B$ is associated with exactly one quantum state. It is, in fact, a quantum analog of the first Newton law of dynamics. A *rarefied band* correspond to a distribution, in which one quantum state corresponds to a subset B_0 of the Brillouin zone B, whereas the complement $B \setminus B_0$ carries no state.
The Heisenberg model of a magnet with a finite set X of nodes yields rarefied bands, carried by subsets [4]

$$B_0 = B|\kappa = \{\xi\kappa \in B \mid \xi \in \mathbb{Z}\}, \quad \kappa \in K(n). \tag{19}$$

The subset $B|\kappa$ is called a κ-tuply rarefied Brillouin zone. It corresponds to the crystal with $\bar{\kappa} = n/\kappa$ nodes [6]. In particular, $\kappa = 1$ corresponds to a full band.
We notify two important conclusions on the distribution ρ given by Eq. (10): (i) it is *inhomogeneous* in the Brillouin zone B, so that the magnet has to exhibit some rarefied bands (actually, these rarefied bands (19) are labelled by $\kappa \in K(n)$), (ii) the distribution ρ is constant on each generalized star $B^{(\kappa)}$ given by Eq. (17). It is an intrinsic feature of this distribution.
These two conclusions are, in fact, partial results of Weyl's recipe. They reflect the fact that the symmetry of the distribution ρ is determined by the hidden symmetry group Aut C_n.

4 Impurities

Now we assume that the subset $X_0 \subset X$ is occupied by 'host' atoms with the spin s ($m = 2s + 1$), whereas its complement $X' = X \setminus X_0$ is occupied by 'impurities' with the spin $s' \neq s$. Thus

$$X = X_0 \cup X', \tag{20}$$

and, accordingly,

$$n = n_0 + n'. \tag{21}$$

Thus the geometric distribution of nodes is the same as for the homogeneous magnet, and the change consists in chemical occupation. The main difficulty is caused by breaking of translational symmetry C_n of the magnet by impurities, so the notion of the Brillouin zone looses its original meaning.
Let the embedding $X' \subset X$ define the chemical configuration of the magnet (i.e. the distribution of impurities). The set of all magnetic configurations is now

$$\Phi(X' \subset X) = Y_0^{X_0} \times Y'^{X'} \tag{22}$$

and depends on the chemical configuration of the magnet. Hence

$$Y_0 = Y, \quad Y' = \{i \mid i = 1, 2, \ldots, m'\}, \quad m' = 2s' + 1. \tag{23}$$

The notion of quasimomentum and the Brillouin zone is restored by introducing *the ensemble of magnets*, with the extended set of magnetic configurations

$$\Phi_{\mathrm{ens}} = \bigcup_{\sigma \in C_n} \Phi(\sigma(X') \subset X). \tag{24}$$

Obviously, the set $\Phi(X' \subset X)$ is not closed under the action of the group C_n, whereas the set Φ_{ens} already is. The corresponding action $P_{\mathrm{ens}} : C_n \times \Phi_{\mathrm{ens}} \to \Phi_{\mathrm{ens}}$ can be decomposed as

$$P_{\mathrm{ens}} \cong \bigoplus_{k \in B} m(P_{\mathrm{ens}}, k)\Gamma_k, \tag{25}$$

defining thus the average distribution $\rho_{\mathrm{av}} : B \to \mathbb{Q}$ for the ensemble as

$$\rho_{\mathrm{av}}(k) = m(P_{\mathrm{ens}}, k)/n, \quad k \in B, \tag{26}$$

with $\mathbb{Q}$ being the field of rational numbers.
For the case of single impurity, i.e. $n' = |X'| = 1$, we obtain

$$\rho_{\mathrm{av}} = \frac{m^{n-1}m'}{n}, \quad k \in B. \tag{27}$$

This distribution is thus homogeneous in the Brillouin zone. This result is apparently puzzling, since the translational symmetry of the homogeneous magnet yields an inhomogeneity of the distribution ρ (cf. Eq. (10)), whereas breaking of this symmetry by a single impurity implies a homogeneous distribution ρ_{av} (cf. Eq. (27)). Thus it looks that breaking of magnet symmetry increases the symmetry of quantum state distribution in the Brillouin zone. Actually, this effect should be attributed to the procedure of averaging over the ensemble, rather than breaking of translational symmetry.
We conclude that average over the ensemble of magnets differing mutually by the position of a single impurity (i) restores the quantum number k of quasimomentum and the Brillouin zone, (ii) wipes out the inhomogeneity of the distribution ρ, (iii) preserves the hidden symmetry $\mathrm{Aut}\, C_n$. In particular, ρ_{av} remains constant on each generalized star $B^{(\kappa)}$, $\kappa \in K(n)$.
In general, the distribution ρ_{av} can be inhomogeneous even under average over positions of impurities. The key observation is that rarefied bands emerge from irregular orbits of the action P_{ens} of the translation group C_n on the set Φ_{ens} of all magnetic configurations of the ensemble of magnets.
Let $\mathcal{O} \subset \Phi_{\mathrm{ens}}$ be an orbit with

$$|\mathcal{O}| = \bar{\kappa} = n/\kappa \tag{28}$$

elements, i.e. with the stabilizer $C_\kappa \lhd C_n$. Then the restriction of P_{ens} to this orbit decomposes as

$$P_{\mathrm{ens}}|_{\mathrm{lc}_{\mathbb{C}}\mathcal{O}} \cong \bigoplus_{k \in B|\kappa} \Gamma_k, \tag{29}$$

Table 1: Distribution of states for $n = 6$, $n' = 2$

	$B^{(0)}$	$B^{(1)}$	$B^{(2)}$	$B^{(3)}$
full bands	138	138	138	138
rarefied bands	12	—	12	—
ρ_{av}	25	23	25	23

where the set $B|\kappa$ is the κ-tuply rarefied Brillouin zone (cf. Eq. (19)). In particular, for a regular orbit we have $\kappa = 1$, so that

$$|\mathcal{O}_{\text{reg}}| = n \tag{30}$$

and

$$P_{\text{ens}}|_{\mathbb{1C}_{\mathbb{C}}\mathcal{O}_{\text{reg}}} \cong \bigoplus_{k\in B} \Gamma_k, \tag{31}$$

since $B|1 = B$. Thus each regular orbit yields a full band. For $\kappa > 1$ we have

$$|B|\kappa| < n, \tag{32}$$

so that each regular orbit yields a rarefied band, and thus inhomogeneity of the distribution ρ_{av}.
In the case of two impurities, i.e. $n' = 2$, we have

$$(S_{n-2} \times S_2) \cap C_n = \begin{cases} C_2 & \text{for antipodal impurities } (n \text{ even, } S_2 \subset C_n), \\ C_1 & \text{otherwise,} \end{cases} \tag{33}$$

so that for the case of antipodal impurities the translational symmetry of the magnet is broken only partially (from C_n to C_2).
E.g. for $n = 6$ and $n' = 2$, with the host spin $s = 1/2$ $(m = 2)$ and the impurity spin $s' = 1$ $(m = 3)$, we get

$$|\underline{2}^{\underline{4}} \times \underline{3}^{\underline{2}}| = 2^4 \cdot 3^2 = 16 \cdot 9 = 144 \tag{34}$$

magnetic configurations for a given chemical configuration, i.e. for a given distribution of the two impurities. The total number of magnetic configurations for the ensemble is

$$|\Phi_{\text{ens}}| = 6 \cdot 144 = 864. \tag{35}$$

When the translational symmetry is totally broken, we get a homogeneous distribution. In the case of antipodal impurities the action P_{ens} yields

138	regular orbits of C_6, i.e.	828 configurations
12	irregular orbits of C_6, i.e.	36 configurations
150	orbits	864 configurations

The Brillouin zone decomposes into generalized stars as

$$B = \{0\}, \{\pm 1\}, \{\pm 2\}, \{3\}. \tag{36}$$

The resulting distribution of states is given in Table 1. Rarefied bands emerge from irregular orbits corresponding to the rarefied Brillouin zone

$$B|2 = \{0\}, \{\pm 2\}. \tag{37}$$

5 Conclusions

We have found that impurities break the obvious symmetry of the recipe of Weyl, but preserve the hidden symmetry. As a result, the distribution of quantum states over the Brillouin zone does not loose the hidden symmetry. In particular, it remains constant on each generalized star. Moreover, the procedure of averaging over the ensemble of magnets with translationally equivalent distributions of impurities wipes out, partially or totally, inhomogeneities of thus distribution. Rarefied bands emerge as a result of irregular orbits of translation group action on the set of all magnetic configurations of an ensemble of magnets.

References

[1] H. Weyl, *Symmetry*, Princeton U.P., New Jersey 1952, pp. 119–145.

[2] M. Mucha, *Hidden Symmetries and Weyl's recipe*, in: W. Florek, T. Lulek, and M. Mucha (Eds.), *Symmetry and Structural Properties of Condensed Matter*, World Sci., Singapore 1991, p. 19.

[3] W. Florek and T. Lulek, *Symmetry properties of the density of states in the Brillouin zone for a one-dimensional periodic Heisenberg magnet*, J. Phys. A (Math. Gen.) **20** (1987) 1921.

[4] B. Lulek, *Rarefied bands within the Heisenberg model of magnetism*, in: W. Florek, T. Lulek, and M. Mucha (Eds.), *Symmetry and Structural Properties of Condensed Matter*, World Sci., Singapore 1991, p. 131.

[5] B. Lulek, *Density of states in the Brillouin zone for a finite magnetic linear chain with a single impurity*, Acta Phys. Pol. **A74** (1988) 453.

[6] M. Kuźma, *Fractal symmetries of line polymers*, in: W. Florek, T. Lulek, and M. Mucha (Eds.), *Symmetry and Structural Properties of Condensed Matter*, World Sci., Singapore 1991, p. 379.

[7] T. Lulek, *Density of states in the reciprocal lattice for a one-dimensional periodic Heisenberg magnet*, J. Physique **45** (1984) 29.

[8] H.O. Foulkes, *Characters of symmetric groups induced by characters of cyclic subgroups*, Proc. Conf. Combinatorial Mathematics, Mathematical Institute, Oxford 1972, p. 141.

[9] A. Kerber, B. Lulek, T. Lulek, *Group actions, configurations and finite states*, in: W. Florek, T. Lulek, and M. Mucha (Eds.), *Symmetry and Structural Properties of Condensed Matter*, World Sci., Singapore 1991, p. 3.

ADDRESS OF THE AUTHOR:
B.Lulek
Division of Mathematical Physics
The Institute of Physics
A.Mickiewicz University
Matejki 48/49
60-769 Poznań, Poland