Density of states in the reciprocal lattice for a one-dimensional periodic Heisenberg magnet

T. Lulek

To cite this version:
T. Lulek. Density of states in the reciprocal lattice for a one-dimensional periodic Heisenberg magnet. Journal de Physique, 1984, 45 (1), pp.29-34. <10.1051/jphys:0198400450102900>. <jpa-00209737>

HAL Id: jpa-00209737
https://hal.archives-ouvertes.fr/jpa-00209737
Submitted on 1 Jan 1984

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
Density of states in the reciprocal lattice for a one-dimensional periodic Heisenberg magnet

T. Lulek
Institute of Physics, A. Mickiewicz University, Matejki 48/49, 60-769 Poznań, Poland

(Reçu le 13 avril 1983, révisé le 3 août, accepté le 12 septembre 1983)

1. Introduction.

According to a common assumption in solid state theory, all elementary excitations in a crystal, including magnons, can be described in terms of quasiparticles (cf. e.g. Kittel [1], or Mattis [2]). It means, in terms of band theory, that the energies of these excitations, as well as the corresponding quantum states, can be completely classified by means of two sets of quantum numbers : the wave vector $k$ from the first Brillouin zone $B$ (kinematical variables) and the band index $A$ (internal variables), and that the excitation energy is a quasiconstant function of $k$, where an admissible value of $k \in B$ is associated with exactly one quantum state within each $A$. Assuming the cyclic periodic Born-Karman boundary conditions, that is, using the model of a crystal, which is periodic in three dimensions, one gets that the density of states in the reciprocal lattice for any band is constant and equal to $N/V_B$ for a sc lattice with the lattice constant $a$), where $N = N_1 N_2 N_3$ is the number of elementary cells for the crystal with periods $N_1$, $N_2$, $N_3$, and $V_B$ is the volume of the first Brillouin zone $B$.

In particular, this kind of homogeneous density of states in the reciprocal lattice is a characteristic property of a quasiparticle without internal degrees of freedom, since the quasimomentum $k$ for such a quasiparticle constitutes the complete set of commuting observables. More generally, for a quasiparticle with internal degrees of freedom (e.g. the spin of an electron, the polarization of a phonon, etc.) the complete set of commuting observables consists of all pairs $(k, A)$, with $k$ ranging over the whole $B$ for each $A$. However, there is no justified a priori reason why any elementary excitation in a crystal should be a quasiparticle, with the spectrum consisting of full bands. In particular, one cannot eliminate the possibility that, for some elementary excitations, certain values of $k$ are forbidden for some $A$'s. Evidently, such excitations would form some « rarefied »
bands $A$, associated only with a subset $B'$ of the Brillouin zone $B$ consisting of those $k \in B$ for which the pair $(k, A)$ is not forbidden. Such excitations cannot be considered as quasiparticles.

In the model of a periodic Heisenberg magnet, one considers the system consisting of $N$ spins $s$, localized on lattice nodes, and interacting pairwise by exchange forces. The ground state of such a magnet, as well as excited states (e.g. those corresponding to magnons) should be vectors belonging to $(2s+1)^N$-dimensional Hilbert space $L^N$, being the simple product of $N$ copies of a one-site space $L$ spanned on states $\{|sm> | m = -s, -s+1, ..., s\}$ corresponding to the admissible projections of the spin onto a given axis. It is by no means evident whether the space $L^N$ can be decomposed in any natural way into $N$-dimensional subspaces corresponding to bands. Contrarily, even some very simple arguments from number theory show that the dimension $(2s+1)^N$ is frequently not divisible by $N$, especially for small $s$ and large $N$ (e.g. for $s = 1/2$ one gets the number $2^N$, which is not divisible by any $N$ different from a power of 2). One can therefore expect some inhomogeneity of the density of states in the reciprocal lattice for this model. The aim of this paper is to explicitly determine the global density of states in the reciprocal lattice for the model of a one-dimensional periodic Heisenberg magnet, i.e. to find the function $\rho(k)$, giving the number of linearly independent states in the space $L^N$ with the wave number $k \in B$.

A rigorous formulation, as well as a solution of the above problem can be provided by means of the theory of groups, in particular by irreducible and permutation representations for finite groups (e.g. Hamermesh [3], Curtis and Reiner [4], Hall [5]), together with an application of the combinatorial analysis (e.g. Hall [6]) and some elements of the number theory (Hasse [7]). A group — theoretical formulation of the problem is given in section 2, a solution — in section 3, a few examples — in section 4, and a discussion — in section 5.

2. Formulation of the problem.

2.1 THE DISTRIBUTION OF MAGNETIC SITES. — The sites of a one-dimensional periodic Heisenberg magnet form, by definition, a closed linear chain constituting an orbit

$$\Delta_N = \{ j | j = 1, 2, ..., N \}$$

of the regular representation of the translation group $T$, isomorphic with the cyclic group $C_N$. The elements of $T$ will be labelled by the numbers of sites $j \in \Delta_N$, and the multiplication in $T$ is the addition modulo $N$. We assume therefore, for the sake of simplicity, that the one-dimensional « elementary cell » of the chain contains one site.

The translation group $T$ is a subgroup of the group $\Sigma_N$ of all permutations on the orbit $\Delta_N$.

Let

$$\sigma = \left( \begin{array}{c} j \\ \sigma(j) \end{array} \right) \in \Sigma_N , \quad j \in \Delta_N$$

be an arbitrary element of the group $\Sigma_N$ on the block $\Delta_N$, $\sigma(j)$ and $\bar{\sigma}(j)$ being respectively the image and the counter-image of the element $j \in \Delta_N$ under the permutation $\sigma$. Equation 2 determines a « natural » permutation representation $W$ of the group $\Sigma_N$ on the set $\Delta_N$, if one identifies $\sigma$ with $W(\sigma)$. The restriction $W|_T$ of the representation $W$ to the subgroup $T \subset \Sigma_N$ is the transitive regular representation of the group $T$, which decomposes into irreducible representations $\Gamma_k$ of $T$, labelled with the wave number $k$ belonging to the one-dimensional first Brillouin zone $B = \{ k | k = 0, \pm 1, \pm 2, ... \}$. Equation 2 according to a formula

$$W|_T = \sum_{k \in \Delta} \Gamma_k.$$ (4)

2.2 THE SPACE OF STATES OF THE MAGNET. — Let

$$\tilde{s} = \{ m | m = -s, -s+1, ..., s \}$$

denotes the set of all admissible projections $m$ of a one-site spin onto a given axis, and $|\tilde{s}| = 2s+1$ — the number of elements of the set $\tilde{s}$. Let $|sm >$ be a standard spin eigenstate on the site $j$. The Hilbert space $L^N$ of states of the magnetic linear chain is spanned on the orthonormal basis of vectors

$$|m_1, ..., m_N > = \prod_{j \in \Delta_N} |sm_j >_j ,$$ (6)

which are in a one-to-one correspondence with elements of the set

$$\tilde{s}^N = \{ (m_1, ..., m_N) | m_j \in \tilde{s} \quad \text{for} \quad j \in \Delta_N \} ; \quad |\tilde{s}^N| = |\tilde{s}|^N.$$ (7)

2.3 THE PERMUTATION REPRESENTATION IN $L^N$ AND THE DENSITY OF STATES IN THE RECIPROCAL LATTICE. — It is a straightforward matter to show that the set of operators $P(\sigma), \sigma \in \Sigma_N$, defined by the formula

$$P(\sigma) |m_1, ..., m_N > = |m_{\sigma(1)}, ..., m_{\sigma(N)} > ,$$ (8)

where $\sigma$ is given by equation 2, forms a linear representation $P$ of the group $\Sigma_N$ in the space $L^N$. $P$ is also the permutation representation of $\Sigma_N$ on the set $\tilde{s}^N$. The restriction $P|_T$ of this representation to the subgroup $T \subset \Sigma_N$ decomposes into irreducible representations $\Gamma_k$ of $T$. The density of states in the reciprocal lattice can be thus defined (up to a constant factor $a/2\pi$, with $a$ — the lattice constant) as the mapping $\rho : B = Z (Z$ is the ring of integers), with $\rho(k)$ being the
multiplicity of $\Gamma_k$ in the restriction $P|_T$. The aim of this paper is to find the mapping $\rho$.

3. A solution of the problem.

3.1 General prescription. — A general prescription for the determination of the function $\rho(k)$ is provided by the standard formula from representation theory for finite groups, which in our case reads

$$\rho(k) = \frac{1}{N} \sum_{j \in T} \chi^P(j) e^{-2\pi i k j / N},$$

(9)

where $\chi^P(j)$ is the character of the representation $P$ for the element $\sigma \in \Sigma_N$, labelled by $j$, and $\exp(2\pi i k j / N)$ is the corresponding character of $\Gamma_k$.

3.2 Character of the permutation representation $P$. — We proceed to evaluate the character $\chi^P(\sigma)$ for an arbitrary $\sigma \in \Sigma_N$. By definition it is given by

$$\chi^P(\sigma) = \sum_{(m_1, \ldots, m_N) \in \Sigma^N} |m_1, \ldots, m_N| \left( P(\sigma) \right) |m_1, \ldots, m_N| = \prod_{j \in T} \sum_{m_j \in \Sigma} \delta(m_j, \sigma(m_j)).$$

(10)

Decomposing the permutation $\sigma$ into cycles one easily observes that non-vanishing contributions to the character $\chi^P(\sigma)$ are provided only by those $N$-tuples $(m_1, \ldots, m_N) \in \Sigma^N$, for which $m_j$ is (an arbitrary) constant within each cycle. Moreover, each cycle contributes the factor $|\sigma|$ independently of its lengths. Therefore, denoting

$$v = \{ v_1, v_2, \ldots, v_N \}; \quad \sum_{i=1}^N iv_i = N,$$

(11)

where $v_i$ is the number of cycles with the lengths $i$ in the permutation $\sigma$, one finally obtains

$$\chi^P(\sigma) = |\sigma|^v,$$

(12)

Note that this character is constant within each class of mutually conjugate elements in the symmetric group $\Sigma_N$.

In particular, for the unit element $\sigma_0 \in \Sigma_N$ we have $v_1 = N$, and $v_i = 0$ for $i > 1$, so that we obtain

$$\chi^P(\sigma_0) = |\sigma|^v,$$

(13)

which is the dimension of $L^N$.

In another extreme case, i.e. for the generating element $\sigma_1$ of the group $T$ (corresponding to $j = 1$) we have $v_N = 1$, and $v_i = 0$ for $i < N$, so that

$$\chi^P(\sigma_1) = |\sigma|^v.$$  

(14)

Denoting by $\sigma_j$ the permutation corresponding to an arbitrary element $j \in T$, that is putting

$$\sigma_j = (\sigma_j)^{\text{times}},$$

(15)

we easily observe that $\sigma_j$ decomposes into cycles of the same lengths $\kappa(j)$, equal to the rank of the element $\sigma_j$, i.e.

$$\kappa(j) = \frac{N}{\text{lcd}(N, j)},$$

(16)

where $\text{lcd}(N, j)$ is the largest common divisor of integers $N$ and $j$. Hence we get

$$v_{\kappa(j)} = \text{lcd}(N, j), \quad v_i = 0 \quad \text{for} \quad i \neq \kappa(j),$$

(17)

which yields

$$\chi^P(\sigma_j) = |\sigma|^v_{\kappa(j)} = |\sigma|^v_{\text{lcd}(N, j)}.$$  

(18)

3.3 Final formula. — Using equation 18 and applying some elements of combinatorics (Hall [7], Sec. 2) and number theory (Hasse [7], Chap. 3) one can transform equation 9 to the form

$$\rho(k) = \frac{1}{N} \sum_{\kappa \in K_N} |\sigma|^{v_{\kappa(j)}} \frac{\phi(k)}{\kappa \phi(\text{lcd}(k, k))} k \mu(\frac{k}{\text{lcd}(k, k)}),$$

(19)

where $K_N = \{ \kappa \in Z_+ \mid 1 \leq \kappa \leq N; \text{lcd}(N, N) = \kappa \}$

(20)

is the set of all divisors of the number $N$, $Z_+ = \{ 1, 2, \ldots \}$ being the set of all positive integers, and $\phi : Z_+ \rightarrow Z_+$, and $\mu : Z_+ \rightarrow Z$ is the Euler function ($\phi(n)$ is the number of positive integers which are smaller than, and mutually prime with, $n \in Z_+$) and Möbius function (associated with the so-called algebra of incidences on the set $K_N$, cf. e.g. Hall [6] for details), respectively. If

$$n = \prod_{p \in \pi(n)} p^{v_p(n)}, \quad \sigma_p(n) \in Z_+$$

(21)

is the canonical decomposition of an integer $n$ into prime factors (so that $\pi(n)$ is the set of different prime factors $p > 1$ of $n$), then

$$\phi(n) = n \prod_{p \in \pi(n)} \frac{p - 1}{p},$$

(22)

and

$$\mu(n) = \begin{cases} 1 & \text{for} \quad n = 1, \\ (-1)^{v_p(n)} & \text{if} \quad \sigma_p(n) = 1, \forall p \in \pi(n), \\ 0 & \text{otherwise}. \end{cases}$$

(23)

A derivation of equation 19 is given in the appendix.

It is worthwhile to note that the canonical decomposition (21) allows us to determine uniquely each divisor $\kappa \in K_N$ by a set $\{ \sigma_p(n) \mid p \in \pi(n) \}$ of integral exponents. The set $K_N$ is uniquely determined by constraints

$$0 \leq \sigma_p(\kappa) \leq \sigma_p(N), \quad p \in \pi(N).$$

(24)
In particular, for \( k = 0 (0 \equiv N \mod N) \), that is for the centre of the Brillouin zone one has \( \text{lcm}(k, N) = \kappa \), which yields

\[
\rho(0) = \frac{1}{N} \sum_{\kappa \in K_N} |\hat{\mathbf{r}}|^N \varphi(\kappa).
\] (25)

For \( k = 1 \) one has \( \text{lcm}(k, 1) = 1 \), so that

\[
\rho(1) = \frac{1}{N} \sum_{\hat{\mathbf{r}} \in \pi_N} |\hat{\mathbf{r}}|^N \varphi(\kappa),
\] (26)

where the summation runs over all \( 2^{\text{dim}} \) subsets \( \mathcal{Z} \) of the set \( \pi_N \), and \( \kappa_N = \prod_{p \in \mathcal{P}} p \).

4. Examples.

The simplest non-trivial example is \( N = 2 \), i.e. \( \mathcal{B} = \{ 0, 1 \} \) (this case has been discussed in a previous paper [8]). In this case we have

\[
\rho(0) = \frac{1}{2} (|\hat{\mathbf{r}}|^2 + |\hat{\mathbf{r}}|), \quad \rho(1) = \frac{1}{2} (|\hat{\mathbf{r}}|^2 - |\hat{\mathbf{r}}|),
\] (27)

so that the density of states is larger in the centre of the Brillouin zone (\( k = 0 \)) than on its boundary (\( k = 1 \)). E.g. for \( s = 1/2 \) we have

\[
\rho(0) = 3, \quad \rho(1) = 1,
\] (28)

so that within \( 2^2 = 4 \) states one can form only one «full band» consisting of 2 states, and the other two states are «condensed» at the centre of the Brillouin zone.

For \( N = 3 \), i.e. \( \mathcal{B} = \{ 0, \pm 1 \} \) we have

\[
\rho(0) = \frac{1}{6} (|\hat{\mathbf{r}}|^3 + 2 |\hat{\mathbf{r}}|), \quad \rho(\pm 1) = \frac{1}{6} (|\hat{\mathbf{r}}|^3 - |\hat{\mathbf{r}}|),
\] (29)

and, similarly, for \( N = 5 \), i.e. \( \mathcal{B} = \{ 0, \pm 1, \pm 2 \} \)

\[
\rho(0) = \frac{1}{6} (|\hat{\mathbf{r}}|^5 + 4 |\hat{\mathbf{r}}|), \quad \rho(\pm 1) = \rho(\pm 2) = \frac{1}{6} (|\hat{\mathbf{r}}|^5 - |\hat{\mathbf{r}}|).
\] (30)

We obtain therefore a homogeneous distribution within the whole Brillouin zone, with the exception of its centre.

In general, we obtain such kind of distribution for any prime \( N = p \), i.e. \( \mathcal{B} = \{ 0, \pm 1, \pm 2, \ldots, \pm (p - 1)/2 \} \). In this case

\[
\rho(0) = \frac{1}{p} \left[ |\hat{\mathbf{r}}|^p + (p - 1) |\hat{\mathbf{r}}| \right]
\] (31)

for the centre of the Brillouin zone, and

\[
\rho(k) = \frac{1}{p} \left[ |\hat{\mathbf{r}}|^p - |\hat{\mathbf{r}}| \right] \quad \text{for} \ k \neq 0
\] (32)

outside the centre.

For \( N = 6 \), i.e. \( \mathcal{B} = \{ 0, \pm 1, \pm 2, 3 \} \) we obtain

\[
\rho(0) = \frac{1}{6} (|\hat{\mathbf{r}}|^6 + |\hat{\mathbf{r}}|^3 + 2 |\hat{\mathbf{r}}|^2 + 2 |\hat{\mathbf{r}}|), \quad \rho(\pm 1) = \frac{1}{6} (|\hat{\mathbf{r}}|^6 - |\hat{\mathbf{r}}|^3 - |\hat{\mathbf{r}}|^2 + |\hat{\mathbf{r}}|),
\]

\[
\rho(\pm 2) = \frac{1}{6} (|\hat{\mathbf{r}}|^6 + |\hat{\mathbf{r}}|^3 - |\hat{\mathbf{r}}|^2 - |\hat{\mathbf{r}}|), \quad \rho(3) = \frac{1}{6} (|\hat{\mathbf{r}}|^6 - |\hat{\mathbf{r}}|^3 + 2 |\hat{\mathbf{r}}|^2 - 2 |\hat{\mathbf{r}}|),
\] (33)

a non-trivial inhomogeneity within the Brillouin zone. E.g. for \( s = 1/2 \) we have

\[
\rho(0) = 14, \quad \rho(\pm 1) = 9, \quad \rho(\pm 2) = 11, \quad \rho(3) = 10,
\] (34)

so that, at best, one can form 9 «full» bands, each band enclosing one state for each \( k \in \mathcal{B} \) (6 states for each band), and \( 14 - 9 = 5 « rarefied » bands, one of which exhibits «holes» for \( k = \pm 1 \) (so that \( \mathcal{B}' = \{ 0, \pm 2, 3 \} \); \( |\mathcal{B}'| = 4 \) states, cf. a remark in the Introduction), another — additional «hole» for \( k = 3 \) (\( \mathcal{B}' = \{ 0, \pm 2 \} \); \( |\mathcal{B}'| = 3 \) states), and three other «bands» reduce to the centre of the Brillouin zone (\( \mathcal{B}' = \{ 0 \} \); \( |\mathcal{B}'| = 1 \) state).

5. Discussion.

In the present paper we have derived a general analytical formula (Eq. 19) for the density \( \rho(k) \) of states in the reciprocal lattice for a one-dimensional closed linear chain of \( N \) spins \( s \). In general, it becomes evident that the distribution of \( |\hat{\mathbf{r}}|^n \) states of a finite Heisenberg magnet over the points of the Brillouin zone is never strictly homogeneous, and that the shape of inhomogeneity strongly depends on the arithmetic structure of the integer \( N \), i.e. on its canonical decomposition (21) into prime factors, and in particular, on the set \( \pi_N \) of different prime factors.

In particular, there exists, for an arbitrary \( N \), a «condensation» of states at the centre of the Brillouin zone (\( k = 0 \)), since equations 19 and 25, together with formulae 22 and 23 imply

\[
\rho(0) > \rho(k) \quad \text{for} \ k \neq 0.
\] (35)

In cases when \( N = p \) is a prime integer, equations 31 and 32 imply that \( \rho \) is homogeneous within the whole Brillouin zone, with the exception of the described above condensation at its centre. In other words, one can form within \( |\hat{\mathbf{r}}|^p \) states

\[
l = \left\lfloor \frac{|\hat{\mathbf{r}}|}{p} \right\rfloor (|\hat{\mathbf{r}}|^p - 1) - 1
\] (36)

«full» bands, each containing \( p \) states, and the remaining \( |\hat{\mathbf{r}}| \) states condense at \( k = 0 \).

Integers \( N \) with a more complicated arithmetic structure lead to an inhomogeneity also outside the centre of the Brillouin zone. The possibilities of a formation of «rarefied» bands were demonstrated in section 4 for the case \( N = 6, s = 1/2 \).
One can consider several contributions to the density $\rho(k)$, each corresponding to a particular term in the sum on the right hand side of equation 19, and classified by means of the divisor $\kappa \in K_N$, putting

$$\rho(k) = \sum_{\kappa \in K_N} \rho_\kappa(k), \tag{37}$$

where

$$\rho_\kappa(k) = \frac{1}{N} |\bar{s}|^{N\kappa} w(k, \kappa), \tag{38}$$

and the function $w(k, \kappa)$ is given by equation A.15.

Then the function $w(k, \kappa)$ satisfies the following sum rules

$$\sum_{k \in B} w(k, \kappa) = N \delta_{\kappa, 1}, \tag{39}$$

and

$$\sum_{\kappa \in K_N} w(k, \kappa) = N \delta_{\kappa, 0}. \tag{40}$$

These rules can be easily derived using the form (A.6) for the function $w(k, \kappa)$. The rule (40) is a generalization of equation A.8. Moreover, we have an evident global sum rule

$$\sum_{k \in B} \rho(k) = |\bar{s}|^N. \tag{41}$$

We proceed to discuss the behaviour of the considered density of states for large $N$, i.e. to study some aspects of a «thermodynamic limit». To this aim, we put

$$\rho(k) = \rho_0 + \rho'(k), \tag{42}$$

where

$$\rho_0 = \frac{1}{N} |\bar{s}|^N \tag{43}$$

is the arithmetic mean value over the Brillouin zone, and $\rho'(k)$ is an immediate measure of inhomogeneity. Observing that, using the notation of equation 37, we have

$$\rho_1(k) = \rho_0 \quad \forall k \in B, \tag{44}$$

we are entitled to consider $\rho_0$ as the principal contribution to the density of states for each point of the Brillouin zone. Now we make an estimation

$$\frac{\rho'(k)}{\rho_0} \leq \sum_{1 \neq \kappa \in K_N} |\bar{s}|^{N\kappa/2} w(k, \kappa) \leq \sum_{1 \neq \kappa \in K_N} |\bar{s}|^{N\kappa/2} N \rightarrow 0 \quad \text{for} \quad N \rightarrow \infty, \tag{45}$$

where $\kappa_{\text{min}}$ is the smallest divisor in $K_N$, larger than 1. It follows that the relative inhomogeneity $\rho'(k)/\rho_0$ of the density of states in the reciprocal lattice vanishes in the thermodynamic limit.

It is worthwhile, however, to note that the above estimation does not exclude a situation when the inhomogeneity considered here can be important in the determination of the thermodynamic properties of a magnet. A full study requires knowledge of the spectrum of a Hamiltonian for a magnet, which exceeds the purpose of the present paper. Here, we restrict ourselves to a rough discussion of some possible a priori situations. Suppose that the magnet does not exhibit in its ground state any «spontaneous» breaking of the translational symmetry i.e. the symmetry associated with the group $T$, so that the ground state belongs to the centre of the Brillouin zone. If such a ground state possesses an extension to a «full» band, then the low lying states form an ordinary, acoustic branch. If, however, this ground state belongs to a «rarefied» band, then the low-lying states form a branch with «holes», corresponding to forbidden values of the quasimomentum $k$. Excitations associated with such a branch are not quasiparticles. In particular, if the ground state is a single state, condensed at the centre of the Brillouin zone, then there appears, a gap in the spectrum of low-lying excitations. We end with the remark that equation 39 implies that in principle one can construct for arbitrary $N$ such a Hamiltonian for which the ground state belongs to a «rarefied» band, so that the elementary excitations are not quasiparticles.

Acknowledgments.

This work has been carried out under project No. MR.1.4.11-1, coordinated by the Institute of Physics of the Polish Academy of Sciences, Warsaw.

Appendix

DERIVATION OF FORMULA 19. — We begin with an observation that according to equation 18 the character $\chi_\kappa(j)$ depends only on $\kappa(j)$, the rank of the element $j$ in the additive cyclic group $T \cong \mathbb{Z}/N$ of reminders mod $N$. The summation over the group manifold $A_N$ in equation 9 can be therefore simplified using a decomposition

$$A_N = \bigcup_{\kappa \in K_N} A^{(\kappa)}_N, \tag{A.1}$$

where

$$A^{(\kappa)}_N = \left\{ \xi \frac{N}{\kappa} \mid 1 \leq \xi \leq \kappa; \text{gcd}(\xi, \kappa) = 1 \right\}. \tag{A.2}$$

is the set of elements of rank $\kappa$ in the group $C_N$. Evidently, each two distinct sets $A^{(\kappa)}_N$ and $A^{(\kappa')}_N$ are disjoint and

$$|A^{(\kappa)}_N| = \varphi(\kappa), \tag{A.3}$$

where $\varphi: \mathbb{Z} \to \mathbb{Z}$ is the Euler function 22. Accordingly,

$$\rho(k) = \frac{1}{N} \sum_{\kappa \in K_N} |\bar{s}|^{N\kappa} w_N(k, \kappa), \tag{A.4}$$
where
\[ w_N(k, \kappa) = \sum_{j \in \mathbb{D}_N} e^{2\pi i j/\kappa} N. \] (A.5)

Substituting \( j \) by \( jN/\kappa \) according to equation A.2 one finds that the function \( w_N(k, \kappa) \) is independent on \( N \) since
\[ w_N(k, \kappa) = \sum_{\xi \in \mathbb{D}_k} e^{2\pi i j/\kappa} N = w(k, \kappa). \] (A.6)

Let us first consider the case \( k = 1 \), corresponding to the irreducible representation, which generates all other irreducible representations of the group \( C_N \) as its simple powers. An elementary property of the set of all complex \( N \)th degree roots of unity
\[ \sum_{j \in \mathbb{D}_N} e^{2\pi i j/\kappa} N = 0 \text{ for } N > 1 \] (A.7)
takes in our notation the form
\[ \sum_{\kappa \in \mathbb{K}_N} w(1, \kappa) = 0 \text{ for } N > 1, \] (A.8)
which together with an evident boundary condition
\[ w(1, 1) = 1 \] (A.9)
allows to determine the function \( w(1, \kappa) \) recursively. E.g., choosing \( N = p \), where \( p \) is a prime integer, one has \( K_p = \{ 1, p \} \), which yields
\[ w(1, 1) + w(1, p) = 0, \text{ thus } w(1, p) = -1, \] (A.10)
etc. In this way we get that
\[ w(1, \kappa) = \mu(\kappa), \] (A.11)
where \( \mu(\kappa) \) is the Möbius function (23).

Now we proceed to consider the general situation, for an arbitrary \( k \in \mathbb{B} \). The crucial rôle is played by the homomorphism \( \psi_k : C_N \rightarrow C_{\kappa} \) given by
\[ \psi_k(j) = kj \mod N. \] (A.12)

Since
\[ \psi_k \left( \frac{N}{\kappa} \right) = k' \frac{N}{\kappa} \mod N = N \frac{\xi'}{\kappa'} \mod N, \] (A.13)
where
\[ \kappa' = \frac{\kappa}{\text{lcm}(k, \kappa)}, \quad \xi' \in \mathbb{A}(\kappa'), \] (A.14)
it follows that the image of the set \( \mathbb{D}_N^{(\kappa)} \) under the homomorphism \( \psi_k \) is the set \( \mathbb{D}_N^{(\kappa')} \). Moreover, it is a straightforward matter to show that the restriction of the homomorphism \( \psi_k \) to the subset \( \mathbb{D}_N^{(\kappa')} \subset C_N \) is a surjection onto the set \( \mathbb{D}_N^{(\kappa')} \) with \( \kappa' \) given by equation (A.14), and that the counter-image of any \( \xi' \in \mathbb{D}_N^{(\kappa')} \) under this surjection contains \( \varphi(\kappa') \) elements of the set \( \mathbb{D}_N^{(\kappa')} \). The definitions (A.5) and (A.6) imply therefore that
\[ w(k, \kappa) = \frac{\varphi(\kappa') \mu(\kappa')}{\varphi(\kappa')} , \] (A.15)
which yields equation 19, the final formula for the density of states in the reciprocal lattice.

References