On the Theory of Metals.

I. Eigenvalues and eigenfunctions of a linear chain of atoms

H. Bethe in Rome

Zeitschrift für Physik **71** (1931) 205–226.

17 June 1931

Original title:

Zur Theorie der Metalle.
I. Eigenwerte und Eigenfunktionen der linearen Atomkette.

(Translation by T. C. Dorlas, DIAS, 9 November 2009.)

Abstract

A method is described for calculating, to zeroth and first order respectively (in the sense of London and Heitler), the eigenfunctions and eigenvalues for a "one-dimensional metal" consisting of a linear chain of very many atoms, each of which has a single s-electron with spin. Besides Bloch's "spin waves", there exist eigenfunctions where the spins pointing in one direction tend to reside on neighbouring atoms. These eigenfunctions might be of importance for the theory of ferromagnetism.

§1. In the theory of metals, one has so far considered only the movement of single conduction electrons in the field of the metal atoms (Sommerfeld, Bloch). The interaction between the electrons has been ignored, at least to the extent that it could not be included in the potential acting on the electrons. This approach has been very fruitful in treating the problem of metallic conduction (with the exception of superconduction). However, it has not allowed a deeper understanding of the problem of ferromagnetism for example[1], and it has made the calculation of cohesion forces in metals a virtually hopeless task: The exchange forces between the electrons, which are relevant for the size of the first-order terms in the perturbation series

[1]F. Bloch, Zs. f. Phys. **57**, 545 (1929) showed that under certain circumstances, 'free electrons' can also exhibit ferromagnetism.

for the energy, are of the same order of magnitude as the zero-point energy of the electron gas, and one can estimate that the second order is again of this magnitude, etc. This behaviour makes one somewhat sceptical about the entire approximation, in which the movement of the individual electrons (the kinetic zero-point energy) is considered to be of greater importance than the interaction (or exchange) energy.

Therefore, Slater[2] and Bloch[3] have recently attempted to approximate the problem from the opposite side, i.e. assuming that the atoms are fixed and considering the interaction as a perturbation, just as in the London-Heitler approximation for molecules. Slater was especially interested in the cohesion forces in non-ferromagnetic materials, where the London-Heitler exchange integral J is in general negative[4], and he developed an interesting method for the approximate calculation of the ground state energy of such metals, for which the total spin obviously vanishes. Bloch, for the purpose of ferromagnetism, calculated approximately the lowest terms in a systematic fashion in the opposite case where $J > 0$. However, in his method, he obtained too many eigenvalues. It is the aim of the present work to demonstrate, at first in the case of a linear chain of atoms, a method for calculating all eigenvalues of a one-dimensional crystal to arbitrary precision. This arbitrary precision, of course, has to be understood in the framework of the first approximation of the London-Heitler method, so that the problem has the same status as the H_2 molecule in the work of London and Heitler. We obtain, in addition to modified versions of the solutions found by Bloch, a set of solutions of a different type, in such a way that the total number of eigenvalues is exactly the correct one.

§2. Our problem is therefore as follows: Given is a linear chain of very many (N) identical atoms. Each atom has, apart from closed shells, one conduction electron in an s-orbit. We assume that the eigenfunction of the free atoms is known. What are the eigenfunctions to zeroth, and the eigenvalues to first-order approximation of the total system including the interaction between the atoms?

Disregarding the interaction, each atoms has two states with equal energy: the spin of the conduction electron can point to the right or to the left. To zeroth order, the eigenvalue of the chain is therefore 2^N-fold degenerate. A state of the chain can be fixed by indicating for which atoms the spin points to the right. Assume that this is the case at the atoms with numbers $m_1, \ldots, m_r$. Let the corresponding eigenfunction of the chain be $\psi(m_1, \ldots, m_r)$. The

[2]J. C. Slater, Phys. Rev. **35**, 509 (1930).

[3]F. Bloch, Zs. f. Phys. **61**, 206 (1930) (in the following referred to as l.c.).

[4]W. Heisenberg, Zs. f. Phys. **49**, 619 (1928).

correct eigenfunction, in zeroth-order approximation, can then be written in the form

$$\Psi = \sum_{m_1, m_2, \ldots, m_r} a(m_1, m_2, \ldots, m_r)\, \psi(m_1, \ldots, m_r),$$

where the numbers $m_1, \ldots, m_r$ run through the values 1 to N, and we will assume that

$$m_1 < m_2 < \cdots < m_r.$$

If we calculate the matrix elements of the interaction energy w.r.t. the states defined by the spin distributions $m_1, \ldots, m_r$, then we obtain the following[5]:

Diagonal elements: If the spin distribution $m_1, \ldots, m_r$ contains N' neighbouring pairs of parallel spins, then

$$W_{m_1, \ldots m_r,\, m_1 \ldots m_r} = E_0 - N'J.$$

E_0 is the interaction due to the charged clouds of the atoms; J is the London-Heitler exchange integral between neighbouring atoms. For non-nearest neighbour atoms we neglect the exchange integral because it decreases exponentially in the distance.

Non-diagonal elements: These occur between two states which can be obtained from one another by exchanging two nearest-neighbour spins with opposite spins. For example, in our notation, the states $m_1 \ldots m_i \ldots m_r$, and $m_1 \ldots m_i + 1 \ldots m_r$, where it is assumed that $m_i + 1$ is indeed a left-pointing spin, i.e. $m_{i+1} \neq m_i + 1$. All such off-diagonal elements of the interaction energy are equal to $-J$.

Using these matrix elements for the interaction energy, we obtain the following equations between the coefficients $a(m_1 \ldots m_r)$ of the required eigenfunction Ψ:

$$2\epsilon a(m_1 \ldots m_r) + \sum_{m'_1 \ldots m'_r} [a(m'_1 \ldots m'_r) - a(m_1 \ \ldots m_r)] = 0. \tag{1}$$

Here

$$2\epsilon J = e - E_0 + NJ, \tag{2}$$

e being the total perturbed energy to first approximation. The sum runs over all distributions $m'_1 \ldots m'_r$ that can be obtained from $m_1 \ldots m_r$ by exchanging neighbouring opposite spins[6].

[5] F. Bloch, l.c.

[6] The equation (1) is due to Bloch, l.c., more accurately derived [there Eqn. (5)]; the atoms are numbered with f_i there instead of m_i, and instead of $2\epsilon J$, he writes simply ϵ.

Apart from the equation (1), the coefficients a should also satisfy the periodicity condition

$$a(m_1 \dots m_i \dots m_r) = a(m_1 \dots m_i + N \dots m_r). \tag{3}$$

§3. For $r = 1$, the solution of (1) reads, as is well-known,

$$\begin{aligned} a(m) &= e^{ikm}, \\ \epsilon &= 1 - \cos k, \\ k &= \frac{2\pi}{N}\lambda,\ \lambda = \text{integer}. \end{aligned}$$

For $r = 2$ we have to distinguish two cases: Either the two right-spins are separate from one another, in which case

$$\begin{aligned} -2\,\epsilon\, a(m_1 m_2) &= a(m_1+1, m_2) + a(m_1-1, m_2) + a(m_1, m_2+1) \\ &\quad + a(m_1, m_2-1) - 4a(m_1, m_2) \quad (m_2 \neq m_1 + 1), \end{aligned} \tag{4-a}$$

or they are nearest neighbours:

$$\begin{aligned} -2\,\epsilon\, a(m_1, m_1+1) &= a(m_1-1, m_1+1) + a(m_1, m_1+2) \\ &\quad -2a(m_1, m_1+1). \end{aligned} \tag{4-b}$$

The first group of equations is solved rigorously by setting

$$\begin{aligned} a(m_1 m_2) &= c_1 e^{i(f_1 m_1 + f_2 m_2)} + c_2 e^{i(f_2 m_1 + f_1 m_2)}, \\ \epsilon &= 1 - \cos f_1 + 1 - \cos f_2, \end{aligned} \tag{5}$$

where the constants c_1, c_2, f_1, f_2 are for the moment undetermined.

The second group can be satisfied by choosing c_1 and c_2 such that

$$0 = a(m_1 m_2) + a(m_1+1, m_1+1) - 2a(m_1, m_1+1). \tag{6}$$

Here, $a(m_1, m_1)$ has no physical meaning, but is defined by (5). Clearly, by adding (6) to (4-b), it becomes of the form (4-a), which has already been solved. Inserting (5) into (6) gives

$$e^{i(f_1+f_2)m_1}[c_1(1 + e^{i(f_1+f_2)} - 2e^{if_2}) + c_2(1 + e^{i(f_1+f_2)} - 2e^{if_1})] = 0, \tag{7}$$

$$\frac{c_1}{c_2} = -\frac{\cos\frac{f_1+f_2}{2} - e^{i\frac{f_1-f_2}{2}}}{\cos\frac{f_1+f_2}{2} - e^{-i\frac{f_1-f_2}{2}}} = \frac{\sin\frac{f_1-f_2}{2} + i\left(\cos\frac{f_1+f_2}{2} - \cos\frac{f_1-f_2}{2}\right)}{\sin\frac{f_1-f_2}{2} - i\left(\cos\frac{f_1+f_2}{2} - \cos\frac{f_1-f_2}{2}\right)}.$$

We set $c_1 = e^{i\varphi/2}$ and $c_2 = e^{-i\varphi/2}$, so that

$$\cot\frac{\varphi}{2} = \frac{\sin\frac{f_1-f_2}{2}}{\cos\frac{f_1+f_2}{2} - \cos\frac{f_1-f_2}{2}},$$

$$2\cot\frac{\varphi}{2} = \cot\frac{f_1}{2} - \cot\frac{f_2}{2}. \tag{8}$$

Correspondingly,

$$a(m_1, m_2) = e^{i(f_1 m_1 + f_2 m_2 + \frac{1}{2}\varphi)} + e^{i(f_2 m_1 + f_1 m_2 - \frac{1}{2}\varphi)}. \tag{9}$$

Here it is assumed that m_1 and m_2 are in the basic part of the chain, i.e. $1 \leq m_1 < m_2 \leq N$. The periodicity condition requires:

$$a(m_1, m_2) = a(m_2, m_1 + N). \tag{10}$$

[The notation $a(m_2, m_1 + N)$ is suggested by the fact that we want to order the m_i according to their size; *cf.* above.] Inserting (9) into (10),

$$\begin{aligned} & e^{i(f_1 m_1 + f_2 m_2 + \frac{1}{2}\varphi)} + e^{i(f_2 m_1 + f_1 m_2 - \frac{1}{2}\varphi)} \\ = \;& e^{i(f_1 m_2 + f_2(m_1+N) + \frac{1}{2}\varphi)} + e^{i(f_2 m_2 + f_1(m_1+N) - \frac{1}{2}\varphi)}. \end{aligned}$$

Since this has to hold for all m_1 and m_2, the first summand on the left must equal the second on the right and vice versa, so that

$$\begin{aligned} N f_1 - \varphi &= 2\pi\lambda_1, \\ N f_2 + \varphi &= 2\pi\lambda_2, \\ \lambda_1, \lambda_2 &= 0, 1, 2, \ldots, N-1. \end{aligned} \tag{11}$$

The numbers f_1 and f_2 do not have the usual form $\frac{2\pi}{N}\lambda$, but their sum does:

$$k = f_1 + f_2 = \frac{2\pi}{N}(\lambda_1 + \lambda_2). \tag{12}$$

k is a true integration constant of the problem; the coefficient $a(m_1, m_2)$ is multiplied by e^{ik} when both right-spins are moved one place to the right, which obviously does not affect the physics of the system.

We presently discuss the behaviour of the phase φ as a function of f_1 and f_2, where we take the convention that

$$-\pi \leq \varphi \leq \pi. \tag{13}$$

Interchanging f_1 and f_2 obviously leads to a change of sign for φ, while the coefficients a remain unchanged according to (9). If we keep f_2 fixed and

let f_1 increase starting at zero, then $\cot(\varphi/2)$ decreases from $+\infty$ to smaller positive values, reaching 0 when $f_1 = f_2$; φ therefore increases from 0 to π. As f_1 becomes slightly bigger than f_2, φ jumps from $+\pi$ to $-\pi$, and then increases steadily back to 0 when f_1 increases further to 2π. If $f_1 = f_2$ then either

$$\varphi = +\pi, \quad \lambda_1 = \lambda_2 - 1 = \frac{N f_1}{2\pi} - \frac{1}{2},$$

or

$$\varphi = -\pi, \quad \lambda_1 = \lambda_2 + 1 = \frac{N f_1}{2\pi} + \frac{1}{2}.$$

In both cases, we have, according to (9), for all m_1, m_2,

$$a(m_1, m_2) = e^{i f_1 (m_1 + m_2)} \left(e^{i\frac{\pi}{2}} + e^{-i\frac{\pi}{2}} \right) = 0.$$

Conclusion: $f_1 = f_2$ *does not lead* to a meaningful solution of the problem, and for a given λ_2, λ_1 can only take the values

$$\lambda_1 = 0, 1, \ldots, \lambda_2 - 2, \lambda_2 + 2, \ldots, N - 1.$$

Moreover, since f_1, f_2 and f_2, f_1 yield the same solution, we may assume $f_1 < f_2$. Thus, for a given λ_2, there are $\lambda_2 - 1$ solutions $\lambda_1 = 0, 1, \ldots, \lambda_2 - 2$, and λ_2 runs from 2 to $N - 1$, so the total number of solutions is

$$\sum_{\lambda_2=2}^{N-1} (\lambda_2 - 1) = \begin{pmatrix} N-1 \\ 2 \end{pmatrix}.$$

However, there must clearly be as many solutions as there are spin distributions, i.e. $\binom{N}{2}$. With our more accurate discussion, we have have therefore come to the conclusion that the usual spin waves *do not yield sufficiently many solutions*, whereas Bloch (l.c.) suggested that the method yielded too many solutions, namely $\binom{N+1}{2}$.

§4. There must therefore be a further $N - 1$ solutions. These can be obtained if one allows the wave numbers f_1 and f_2 to have conjugate complex values. Indeed, we will find that, for every arbitrary value of $f_1 + f_2 = k$, one can find exactly one pair of conjugate complex solutions of (8) and (11). Let

$$\left.\begin{array}{ll} f_1 & = u + i\,v, \\ f_2 & = u - i\,v; \end{array}\right\} \tag{14}$$

then

$$\cot\frac{f_1}{2} = \frac{\cos\frac{u}{2}\cosh\frac{v}{2} - i\sin\frac{u}{2}\sinh\frac{v}{2}}{\sin\frac{u}{2}\cosh\frac{v}{2} + i\cos\frac{u}{2}\sinh\frac{v}{2}} = \frac{\sin u - i\sinh v}{\cosh u - \cos u}. \tag{15}$$

Now, by (11),

$$N(f_1 - f_2) = 2N\,i\,v = 2\pi(\lambda_1 - \lambda_2) + 2\varphi,$$

$$\left.\begin{array}{ll} \varphi & = \psi + i\,\chi, \\ \psi & = \pi(\lambda_2 - \lambda_1), \\ \chi & = N\,v. \end{array}\right\} \tag{16}$$

If v should take a finite value (i.e $v > 0$), then χ must be very large, and hence

$$\cot\frac{\varphi}{2} \approx \frac{\sin\psi - \frac{1}{2}ie^{\chi}}{\frac{1}{2}e^{\chi} - \cos\psi} \approx -i + 2e^{-\chi}(\sin\psi - i\cos\psi),$$

$$\cot\frac{\varphi}{2} \approx -i(1 + 2e^{-\chi+i\psi}). \tag{17}$$

To *first* approximation, therefore,

$$\begin{aligned} 2\cot\frac{\varphi}{2} &= \cot\frac{f_1}{2} - \cot\frac{f_2}{2} = -2\,i \\ &= \frac{\sin u - i\sinh v}{\cosh v - \cos u} - \frac{\sin u + i\sinh v}{\cosh v - \cos u}, \end{aligned}$$

$$\sinh v = \cosh v - \cos u,$$

$$e^{-v} = \cos u \tag{18}$$

and

$$\begin{aligned} \epsilon &= 2 - \cos(u + iv) - \cos(u - iv) \\ &= 2 - 2\cos u\cosh v = 2 - \cos u\left(\cos u + \frac{1}{\cos u}\right), \end{aligned}$$

$$\epsilon = \sin^2 u = \tfrac{1}{2}(1 - \cos 2u). \tag{19}$$

Apparently, we must have $\cos u \geq 0$, i.e. $-\frac{\pi}{2} \leq u \leq \frac{\pi}{2}$. Therefore, if $k = 2u + 2n\pi$ (n integer) is given, and

$$\text{between } 0 \text{ and } \pi, \text{then} u = \frac{k}{2},$$

$$\text{between } \pi \text{ and } 2\pi, \text{then } u = \frac{k}{2} - \pi.$$

In the *second* approximation, we set

$$v = v_0 + \epsilon, \tag{20}$$

where v_0 is the value just obtained to first approximation. Then,

$$\begin{aligned} 2\cot\frac{\varphi}{2} &= -2i - 4ie^{-\chi+i\psi} = -2i\frac{\sinh v}{\cosh v - \cos u} \\ &= -2i\frac{\sinh v_0}{\cosh v_0 - \cos u}\left[1+\epsilon\left(\frac{\cosh v_0}{\sinh v_0} - \frac{\sinh v_0}{\cosh v_0 - \cos u}\right)\right] \\ &= -2i\left[1+\epsilon\left(\frac{1+\cos^2 u}{1-\cos^2 u} - 1\right)\right] \\ &= -2i(1+2\epsilon\cot^2 u), \end{aligned}$$

$$\epsilon = \tan^2 u\, e^{-\chi+i\psi}.$$

Since ϵ is in general very small, we can replace χ by $N\,v_0$. ψ is then determined by the given value of k:

If $\frac{N}{2\pi}k = \lambda_1 + \lambda_2 = \lambda$ is even, and smaller than $\frac{N}{2}$, then we can put

$$\lambda_1 = \lambda_2 = \frac{1}{2}\lambda, \quad \psi = 0.$$

Similarly, for $\lambda \geq \frac{N}{2}$ and $N+\lambda$ even,

$$\lambda_1 = \lambda_2 = \frac{1}{2}(-N+\lambda), \quad \psi = 0.$$

If λ resp. $N+\lambda$ is odd, we must write

$$\lambda_2 = \lambda_1 + 1, \quad \psi = \pi.$$

Correspondingly, we have

$$\epsilon = \pm\tan^2 u\, e^{-Nv_0}. \tag{21}$$

For even λ (resp. $N+\lambda$, positive sign), therefore, $v > v_0$; hence, if in the next approximation v_0 is replaced by v then the resulting ϵ is smaller than that in the second approximation; the scheme for calculating v therefore certainly always converges, and even very rapidly. However, if the negative sign has to be taken (for odd λ or $N+\lambda$), then $v < v_0$ and ϵ increases (in absolute value) in subsequent higher approximations. This does not of course make a difference as long as v_0 is finite (i.e. $v_0 > 0$ (ed.)), since ϵ is then only a tiny correction. But if u becomes small, and hence $\cos u \approx 1$, then v_0 also becomes small, and in fact we have, to reasonable accuracy,

$$v_0 = -\log\cos u = 1 - \cos u = \frac{1}{2}u^2.$$

Now, if u is small of order $\frac{1}{\sqrt{N}}$, then Nv_0 is finite, and

$$\epsilon = -u^2\, e^{-Nv_0}$$

is larger in absolute value than v_0 when

$$Nv_0 < \log 2 \approx 0.7, \quad u^2 < \frac{1.4}{N}.$$

For $u < \sqrt{\frac{1.4}{N}}$ and odd λ, therefore, $v_1 = v_0 + \epsilon$ becomes negative, and the scheme diverges. As a result, there is *no* solution with two conjugate complex wave numbers[7].

[In its place there appears an additional solution with two real wave numbers. Again, we consider k as given, so that $f_2 = k - f_1$. Previously, in the discussion about real solutions, we tacidly assumed that with increasing f_1, $F = Nf_1 - \varphi$ also increases monotonically. For, this is rather probable since f_1 is multiplied by such a large factor N, and φ only by 1. Nevertheless, for small k, this increase does not happen. Indeed, we have, using (8),

$$\frac{dF}{df_1} = N - 2\frac{\frac{1}{2}\frac{1}{\sin^2\frac{f_1}{2}}\cdot\frac{1}{2} + \frac{1}{4}\frac{1}{\sin^2\frac{k-f_1}{2}}}{1 + \left(\frac{1}{2}\cot\frac{f_1}{2} - \frac{1}{2}\cot\frac{k-f_1}{2}\right)^2},$$

and if we put $f_1 = f_2 = \frac{k}{2}$, then

$$\frac{dF}{df_1} = N - \frac{1}{\sin^2\frac{f_1}{2}}.$$

This is obviously only positive as long as

$$\sin\frac{f_1}{2} > \frac{1}{\sqrt{N}}.$$

For $k < 4\arcsin\frac{1}{\sqrt{N}} \approx \frac{4}{\sqrt{N}}$, the rise of $F = Nf_1 - \varphi$ as a function of f_1 is interrupted by a drop in the neighbourhood of $f_1 = \frac{k}{2}$. If $\frac{Nk}{2\pi} = \lambda$ is *odd*, then

$$N\frac{k}{2} - \pi = 2\pi\lambda_1 = 2\pi\frac{\lambda - 1}{2},$$

where λ_1 is an integer, and for $\lambda_1 = \frac{\lambda-1}{2}$, $\lambda_2 = \frac{\lambda+1}{2}$ there are *two* solutions of the equations (8) and (11): Apart from $f_1 = f_2$, $\varphi = \pi$, there is a solution $f_1 < f_2$, $\varphi \neq \pi$, for which, in contradistinction from the former, the coefficients (9) remain finite.

[7] If actual fact, this case already occurs for $u < \frac{2}{\sqrt{N}}$: although the second approximation for v is then still positive, the higher approximations push it into the negative.

To actually obtain this solution, we set $f_1 = f - \frac{2\epsilon}{N}$, and replace $\sin f = f$, $\cos f = 1$ and $\cot f = \frac{1}{f}$ because of the small size of f. Then we have

$$2\cot\frac{\varphi}{2} = \frac{2}{f - \frac{2\epsilon}{N}} - \frac{2}{f + \frac{2\epsilon}{N}} = \frac{8\epsilon}{Nf^2}, \tag{8a}$$

$$2\varphi = 2\pi(\lambda_2 - \lambda_1) - N(f_2 - f_1) = 2\pi - 4\epsilon, \tag{11a}$$

$$\cot\frac{\varphi}{2} = \tan\epsilon,$$

$$\frac{\tan\epsilon}{\epsilon} = \frac{4}{Nf^2}. \tag{22}$$

This determines ϵ, where $\epsilon < \frac{\pi}{2}$, and also $\varphi > 0$ and $Nf_1 > 2\pi\lambda_1$.]

We have now determined, for each value of λ, an additional solution with real or complex wave numbers. The highest allowed value for λ is clearly $N-2$ with $\lambda_1 = \lambda_2 = N-1$; for $\lambda = N-1$ we would have $\lambda_2 = N$ which is outside the range of values for λ_i[8].

The coefficients $a(m_1, m_2)$ become, for our complex solutions, according to (9), (12) and (16a),

$$a(m_1, m_2) = e^{iu(m_1+m_2)}\left(e^{v(m_1-m_2+\frac{1}{2}N)} \pm e^{v(m_2-m_1-\frac{1}{2}N)}\right),$$

$$a(m_1, m_2) = e^{iu(m_1+m_2)} \begin{matrix}\cosh \\ \sinh\end{matrix} \left[v\left(\tfrac{1}{2}N - (m_2 - m_1)\right)\right]. \tag{23}$$

Here cosh resp. sinh applies depending on whether λ (resp. $N + \lambda$ for $\lambda > N/2$) is even or odd. It is thus for these solutions most probable that the two right-spins are close together, as the probability $|a(m_1, m_2)|^2$ decreases exponentially in the distance $m_2 - m_1$. The most extreme case occurs for the solution $\lambda = \frac{1}{2}N$, $u = \frac{1}{2}\pi$, $v = \infty$: Here, upon appropriate normalisation,

$$a(m_1, m_2) = \begin{cases} 0 & \text{if } m_2 \neq m_1 + 1, \\ (-1)^{m_1} & \text{if } m_2 = m_1 + 1, \end{cases}$$

so the right-spins are always direct neighbours.

Each eigenvalue ϵ with two complex conjugate wave numbers is, as we shall see shortly, *smaller* than all eigenvalues with the same wave number k and real wave numbers. By (2), the corresponding energy to first order lies *deeper* than all solutions with real wave numbers in case the exchange

[8]The solution $\lambda_1 = N-1$, $\lambda_2 = N$ has already been counted as $\lambda_2 = 0$, $\lambda_1 = N-1$.

integral J is *positive* (*ferromagnetic case*), but *higher* when J is *negative* (*normal case*).

Indeed, for the complex solutions,

$$\epsilon_k = \sin^2 u, \tag{19}$$

and for real solutions

$$\epsilon_k = 1 - \cos f_1 + 1 - \cos(k - f_1). \tag{5}$$

(5) is minimal for

$$\begin{cases} f_1 = \frac{1}{2}k, & \text{if } 0 \leq k \leq \pi, \\ f_1 = \frac{1}{2}k + \pi & \text{if } \pi \leq k \leq 2\pi, \end{cases}$$

so in general for $f_1 = f_2 = u$. The minimum is

$$\epsilon_{\min} = 2(1 - \cos u),$$

so that

$$\frac{\epsilon_k}{\epsilon_{\min}} = \frac{1}{2}(1 + \cos u) \leq 1, \tag{24}$$

where the equality sign only applies if $u = 0$[9]. But this was exactly our claim.

§5. We now turn to the general case of r right-oriented spins. The equations (1) again split into different types:
If among the r spins $m_1, \ldots, m_r$ there are no neighbours, then

$$\begin{aligned} -2\,\epsilon\, a(m_1, \ldots, m_r) = \sum_{i=1}^{r} [a(m_1, \ldots, m_i + 1, \ldots, m_r) \\ + a(m_1, \ldots, m_i - 1, \ldots, m_r) - 2a(m_1, \ldots, m_i, \ldots, m_r)]. \end{aligned} \tag{24-a}$$

If there are two neighbours, say $m_{i+1} = m_i + 1$, then we have instead,

$$\begin{aligned} -2\,\epsilon\, a(m_1, \ldots, m_i, \ldots, m_k, m_k + 1, \ldots, m_r) = a(\ldots m_k - 1, m_k + 1, \ldots) \\ + a(\ldots m_k m_k + 2 \ldots) - 2a(\ldots m_k m_k + 1 \ldots) \\ + \sum_{i \neq k, k+1} [a(\ldots m_i + 1 \ldots) + a(\ldots m_i - 1 \ldots) - 2a(\ldots m_i \ldots)] \end{aligned} \tag{24-b}$$

[9] In fact f_1 can never be exactly equal to f_2 (*cf.* §3), so in truth the $<$-sign always applies.

and analogously for the case of more neighbouring spins. We now make the "Ansatz" (hypothesis)

$$a(m_1 \dots m_r) = \sum_{P=1}^{r!} \exp\left[i \sum_{k=1}^{r} f_{Pk} m_k + \frac{1}{2} i \sum_{k<l} \varphi_{Pk,Pl} \right], \tag{25}$$

$$\epsilon = \sum_{k=1}^{r} [1 - \cos f_k]. \tag{26}$$

P is some permutation of the numbers $1, 2, \dots, r$ and Pk denotes the number that this permutation puts in place of k. This hypothesis clearly satisfies the first set of equations (24-a). The remaining equations will be satisfied by requiring that

$$2a(m_1, \dots, m_k m_k + 1, \dots, m_r) = a(\dots m_k m_k \dots) + a(\dots m_k + 1\, m_k + 1 \dots), \tag{27}$$

where the terms on the right-hand side are defined by (25). (27) must hold for arbitrary multiplets of values $m_1, \dots, m_r$, where arbitrary many m_i are neighbours – provided only that $m_1 < m_2 < \dots < m_r$. Thus all equations (24-b) and those in which the distributions $m_1, \dots, m_r$ have *more than two* neighbouring right-spins are satisfied *simultaneously*. Indeed, these equations are reduced (by the substitution (27)) to the type (24-a), which has already been solved. The equations (27) themselves are satisfied by determining the phases φ from

$$2 \cot \frac{\varphi_{kl}}{2} = \cot \frac{f_k}{2} - \cot \frac{f_l}{2}; \quad -\pi \le \varphi_{kl} \le +\pi. \tag{28}$$

That this is the case can be seen completely analogously to §3.

It remains to consider the periodicity condition

$$a(m_1, m_2, \dots, m_r) = a(m_2, \dots, m_r, m_1 + N)$$

$$\sum_{P} \exp\left[i \sum_{k=1}^{r} f_{Pk} m_k + \frac{1}{2} i \sum_{k<l} \varphi_{Pk,Pl} \right]$$
$$= \sum_{P'} \exp\left[i \left(\sum_{k=2}^{r} f_{P'(k-1)} m_k + f_{P'r}(m_1 + N) + \sum_{k<l} \varphi_{P'k,P'l} \right) \right].$$

This must hold for all $m_1, \dots, m_r$; therefore each pair of terms on the left and right, which depend on the m_k in the same way, must be equal individually.

For example, the term P on the left and the term P'' on the right, where P'' is defined by

$$P''(k-1) = Pk \quad (k = 2, \ldots, r), \quad P''r = P1.$$

This yields

$$\begin{aligned} &Nf_{P''r} + \frac{1}{2}\sum_{k<l} \varphi_{P''k,P''l} - \frac{1}{2}\sum_{k<l} \varphi_{Pk,Pl} = 2\pi\lambda \\ &= Nf_{P1} + \frac{1}{2}\sum_{k<l\le r-1} \varphi_{P(k+1),P(l+1)} + \frac{1}{2}\sum_{k=1}^{r-1} \varphi_{P(k+1),P1} \\ &\qquad - \frac{1}{2}\sum_{2\le k<l} \varphi_{Pk,Pl} - \frac{1}{2}\sum_{k=2}^{r} \varphi_{P1,Pk} \\ &= Nf_{P1} - \sum_{k=2}^{r} \varphi_{P1,Pk}, \end{aligned}$$

where we used the fact that $\varphi_{kl} = -\varphi_{lk}$. Since this holds for all P it follows that

$$Nf_i = 2\pi\lambda_i + \sum_k \varphi_{ik} \tag{29}$$

for all i.

Completely analogously to §3, one can also show that any two f_i can never be equal, as otherwise all coefficients a vanish, and hence that for real f_i two subsequent λ_i must differ by at least two. The number of solutions with real f_i thus becomes

$$\binom{N-r+1}{r}$$

and is therefore much smaller than the required number of solutions $\binom{N}{r}$.

§6. If $f_k = u_k + i\,v_k$ is a complex wave number then it follows from

$$Nf_k = 2\pi\lambda_k + \sum_l \varphi_{kl}$$

that at least one of the φ_{kl} must have a very large imaginary part of the order N. This implies in first approximation (§4)

$$2\cot\tfrac{1}{2}\varphi_{kl} = \cot\tfrac{1}{2}f_k - \cot\tfrac{1}{2}f_l = -2i.$$

There must therefore be a f_l such that the real part of $\cot\frac{1}{2}f_l$ is the same as that of $\cot\frac{1}{2}f_k$, while their imaginary parts differ by $2i$ (up to a quantity of

order e^{-N}). This leads to the following solution, which we shall refer to as a wave complex:

n wave numbers are determined by the identities

$$\cot \tfrac{1}{2} f_\kappa = a - i\,\kappa; \quad \kappa = -(n-1), -(n-3), \ldots, n-1, \tag{30}$$

where a is a constant which is the same for each of the n wave numbers. We then clearly have

$$\varphi_{\kappa,\kappa\pm 2} = \psi \mp i\,\infty,$$

while the other $\varphi_{\kappa,\lambda}$ have a finite imaginary part. ψ remains undetermined. Using (15) we obtain

$$\begin{aligned} \frac{\sin u_\kappa}{\cosh v_\kappa - \cos u_\kappa} &= a, \\ \frac{\sinh v_\kappa}{\cosh v_\kappa - \cos u_\kappa} &= \kappa, \end{aligned}$$

the solutions of which are

$$\begin{cases} u_\kappa = \arctan \frac{2a}{a^2+\kappa^2-1} = \operatorname{arc\,cot} \frac{a}{\kappa+1} - \operatorname{arc\,cot} \frac{a}{\kappa-1}, \\ \operatorname{arctanh} v_\kappa = \frac{2\kappa}{a^2+\kappa^2+1}, \end{cases} \tag{31}$$

$$e^{-2v_\kappa} = \frac{(\kappa+1)^2 + a^2}{(\kappa-1)^2 + a^2}. \tag{32}$$

Here $\sin u$ always has the same sign as a.

We now claim that a can be expressed in terms of the total wave number of the wave complex

$$k = \sum_{\kappa=-(n-1)}^{n-1} f_\kappa = \sum_\kappa u_\kappa \tag{33}$$

in the simple form

$$a = n \cot \tfrac{1}{2} k. \tag{34}$$

For $n = 1$ this is evident, and for $n = 2$ it follows by substitution of the previously obtained solution (18) (*cf.* §4):

$$e^{-v} = \cos u, \quad u = \tfrac{1}{2}k \text{ resp. } \tfrac{1}{2}k + \pi,$$

$$a = \frac{\sin u}{\cosh v - \cos u} = \frac{\sin u}{\frac{1}{2}\left(\frac{1}{\cos u} + \cos u\right) - \cos u} = 2 \cot u = 2 \cot \tfrac{1}{2} k.$$

On the other hand, at constant a, the wave numbers u_κ for a complex of n waves are the same as those for $n-2$ waves; there are simply two additional wave numbers $u_{n-1} = u_{-(n-1)}$, so that

$$\tfrac{1}{2}k_n = \tfrac{1}{2}k_{n-2} + u_{n-1} \tag{33a}$$

If we now assume that (34) has been proven for $n-2$, then we have

$$\begin{aligned} \tfrac{1}{2}k_n &= \operatorname{arc\,cot}\frac{a}{n-2} + \operatorname{arc\,cot}\frac{a}{n} - \operatorname{arc\,cot}\frac{a}{n-2} \\ &= \operatorname{arc\,cot}\frac{a}{n}. \end{aligned}$$

We also claim: The eigenvalue corresponding to our wave complex is

$$\epsilon_n = \frac{1}{n}(1-\cos k). \tag{35}$$

Again, this is obvious for $n=1$, while it was proved in (19) for $n=2$. In general, we have

$$\begin{aligned} \epsilon_n &= \sum_{\kappa=-(n-1)}^{n-1} [1-\cos(u_\kappa + i\,v_\kappa)] \\ &= \epsilon_{n-2} + 2 - \cos(u_{n-1} + i\,v_{n-1}) - \cos(u_{n-1} - i\,v_{n-1}) \\ &= \epsilon_{n-2} + 2\,(1 - \cos u_{n-1}\cosh v_{n-1}) \\ &= \epsilon_{n-2} + 2\left(1 - \frac{[a^2+(n-1)^2-1][a^2+(n-1)^2+1]}{[a^2+(n-1)^2+1]^2 - 4(n-1)^2}\right) \\ &= \epsilon_{n-2} + 4\frac{a^2 - n(n-2)}{(a^2+n^2)(a^2+(n-2)^2)}, \end{aligned}$$

where we have used (31) and (32). If we now assume that (35) is valid for $n-2$, then we get, with the help of (34),

$$\begin{aligned} \tfrac{1}{2}\epsilon_n &= \frac{1}{(n-2)\left(1+\frac{a^2}{(n-2)^2}\right)} + 2\frac{a^2 - n(n-2)}{(a^2+n^2)(a^2+(n-2)^2)} \\ &= \frac{(n-2)(a^2+n^2) + 2(a^2 - n(n-2))}{(a^2+n^2)(a^2+(n-2)^2)} \\ &= \frac{n}{a^2+n^2} = \frac{1}{n}(1-\cos k). \end{aligned}$$

Finally, we want to prove, analogously to §4: Given the number of right-oriented spins r and the total wave number k of all spin waves, the smallest

eigenvalue ϵ is obtained when all r spin waves are combined in a single wave complex. The eigenvalue is then given by

$$\epsilon_r = \frac{1}{r}(1 - \cos k).$$

If, instead, there are two wave complexes with n and $p = r - n$ wave resp., then

$$\epsilon_{p+n} = \frac{1}{n}(1 - \cos k_1) + \frac{1}{p}(1 - \cos(k - k_1)).$$

The minimum of this expression is attained when

$$\frac{1}{n}\sin k_1 = \frac{1}{p} = \sin(k - k_1),$$

$$\sin k_1 = \frac{n \sin k}{\sqrt{n^2 + 2np\cos k + p^2}}.$$

It is

$$\epsilon_{\min} = \frac{n + P - \sqrt{n^2 + p^2 + 2np\cos k}}{n\,p}.$$

Now,

$$(n+p)\sqrt{n^2 + p^2 + 2np\cos k} < (n+p)^2 - np(1 - \cos k),$$

as can be verified easily by squaring. This implies immediately that

$$\epsilon_r < \epsilon_{\min}. \tag{36}$$

If the spin waves constitute more than two wave complexes then ϵ lies even higher of course. The state of lowest energy in case of r right-spins is therefore, when $J > 0$ (ferromagnetic case): *a single* wave complex of r spins; when $J < 0$ (normal case): r separate waves with real wave numbers. Of course, in the latter case, this does not fully determine the lowest energy solution. It is easy to compute the second approximation for the wave numbers of a wave complex, where the u and v in the formulas (31) and (32) are slightly modified to satisfy the true periodicity condition (29). The calculation proceeds in an analogous fashion to §4, and one finds, in general, that for finite k, there is always a solution in the immediate neighbourhood of (31) and (32), whereas for small k of the order $\frac{1}{\sqrt{N}}$, the solution changes its character when $\frac{Nk}{2\pi}$ is not divisible by n. Instead of a complex of three spin waves one then finds, for example, a pair of complex conjugate waves as described in §4 (with even λ), together with a single wave with a real wavenumber in a very close neighbourhood. The total number of solutions is not affected by this transformation in appearance: There is precisely one

solution for each $\lambda = 0, 1, 2, \ldots, N-n$; the latter value corresponding to $\lambda_{-(n-1)} = \lambda_{-(n-3)} = \cdots = \lambda_{n-1} = N-1$. For higher values of λ, one or more λ_κ are equal to N, which is not allowed.

From now on, however, we want to also exclude $\lambda_i = 0$ in general. First of all, we gain in symmetry as a result. Moreover, this automatically separates the solutions for which the *total spin* equals $m = \frac{1}{2}N - r$ from those in which only the left-oriented *component* of the spin has this value, while the total spin itself has a higher value. The latter states, namely, are given precisely by those solutions for which one or more among the r wave numbers equals zero. Thus there remain only $N - 2n + 1$ solutions with a wave complex of n spin waves: $\lambda = n, n+1, \ldots, N-n$.

§7. We now assume that there are *two* wave complexes with n and $p(>n)$ spin waves respectively, and investigate what number of solutions can be obtained this way. For this, we need to discuss the phases φ.

Let the wavenumbers of the first complex be given by

$$\begin{aligned} \cot \tfrac{1}{2} f_\kappa &= a - i\,\kappa, & \kappa &= -(n-1), -(n-3), \ldots, n-1 \\ a &= n \cot \tfrac{1}{2} k_1, & k_1 &= \sum_\kappa f_\kappa, \end{aligned} \tag{37-a}$$

and the second by

$$\begin{aligned} \cot \tfrac{1}{2} f_\mu &= b - i\,\mu, & \mu &= -(p-1), -(p-3), \ldots, p-1 \\ b &= p \cot \tfrac{1}{2} k_2, & k_2 &= \sum_\mu f_\mu. \end{aligned} \tag{37-b}$$

Then we have, by (28), (29) and (31),

$$\begin{aligned} N k_1 &= 2\pi\lambda_1 + \sum_\kappa \sum_\mu \varphi_{\kappa,\mu}, \\ N k_2 &= 2\pi\lambda_2 - \sum_\kappa \sum_\mu \varphi_{\kappa,\mu}, \\ \cot \varphi_{\kappa,\mu} &= \cot(\psi_{\kappa,\mu} + i\,\chi_{\kappa,\mu}) = \frac{1}{2}(a-b) - \frac{1}{2} i(\kappa - \mu), \\ \tan \psi_{\kappa,\mu} &= \frac{a-b}{\frac{1}{4}(a-b)^2 + \frac{1}{4}(\kappa-\mu)^2 - 1}. \end{aligned} \tag{38}$$

Sign of $\psi_{\kappa,\mu}$ = sign of $a-b$, $\sum_\kappa \sum_\mu \chi_{\kappa,\mu} = 0$ since the f_κ and f_μ are arranged in complex-conjugate pairs. The $\psi_{\kappa,\mu}$ are zero when k_1 is very small, a large, and they become positive with increasing k_1 as long as $a > b$. We are particularly interested in its value when a approaches b and eventually becomes smaller

than b, so that we can determine how many values the integers λ_1, λ_2 cannot have. To this end, we keep $\lambda_0 = \frac{Nk_2}{2\pi}$ fixed[10] and define λ' by

$$n \cot \frac{\pi\lambda'}{N} > p \cot \frac{\pi\lambda_0}{N} > n \cot \frac{\pi(\lambda'+1)}{N}. \tag{39}$$

For $Nk_1 = 2\pi\lambda'$, $a - b$ is then clearly still positive, and small of order $1/N$. Hence $\tan \psi_{\kappa,\mu}$ is small and positive when $|\kappa - \mu| > 2$, small and negative when $|\kappa - \mu| < 2$, and very large and positive when $|\kappa - \mu| \approx 2$.

The latter follows from the fact that κ and μ only differ from integers by amount of order $e^{-N} \ll 1/N^2$ (*cf.* §4), so that $\frac{1}{4}(\kappa - \mu)^2 - 1 \ll (a - b)^2$ whenever $|\kappa - \mu|$ is close to 2. We conclude that, up to quantities of order $1/N$,

$$\psi_{\kappa,\mu} = \begin{cases} 0 & \text{for } |\kappa - \mu| > 2, \\ \pi & \text{for } |\kappa - \mu| < 2, \\ \frac{1}{2}\pi & \text{for } |\kappa - \mu| = 2. \end{cases} \tag{40}$$

If we first assume that $p - n$ is *odd*, then, for a given κ, there are exactly two values $\mu = \kappa + 1$ and $\mu = \kappa - 1$, for which $\psi_{\kappa,\mu}$ does not vanish, but has the value π. Hence, in this case

$$\sum_{\kappa} \sum_{\mu} \psi_{\kappa,\mu} = 2\pi n. \tag{41}$$

On the other hand, if $p - n$ is *even*, then, for each κ there exist three μ for which $\psi_{\kappa,\mu} \neq 0$:

$$\begin{aligned} &\mu = \kappa, && \psi_{\kappa,\mu} = \pi, \\ &\mu = \kappa + 2, && \psi_{\kappa,\mu} = \frac{1}{2}\pi, \\ &\mu = \kappa - 2, && \psi_{\kappa,\mu} = \frac{1}{2}\pi. \end{aligned}$$

In total, we have again

$$\sum_{\kappa} \sum_{\mu} \psi_{\kappa,\mu} = 2\pi n.$$

Thus we have

$$\begin{aligned} \lambda_1 &= \frac{Nk_1}{2\pi} - n = \lambda' - n, \\ \lambda_2 &= \lambda_0 + n. \end{aligned} \tag{42-a}$$

[10] We shall see in the following that for $a \approx b$, k_1 and k_2 are indeed of the form $\frac{2\pi}{N}$ times an integer, so that $\lambda_0 =$ an integer.

Similarly, for $Nk_1 = 2\pi(\lambda' + 1)$,

$$\begin{aligned} \sum_\kappa \sum_\mu \psi_{\kappa,\mu} &= -2\pi n, \\ \lambda_1 &= \lambda' + 1 + n, \\ \lambda_2 &= \lambda' - n. \end{aligned} \tag{42-b}$$

The possible values for λ_1 are therefore

$$\lambda_1 = n, n+1, \ldots \lambda' - n, \lambda' + n + 1, \ldots, N - n. \tag{42-c}$$

The $2n$ values $\lambda' - n + 1, \ldots, \lambda' + n$ are forbidden due to the presence of the other spin complex. In the same way one can see that if λ_0 is small then, in general, $b > a$ and hence $\lambda_2 = \lambda_0 - n$. But λ_2 must be at least p (see the end of the previous section), so $\lambda_0 > p + n$. Similarly, $\lambda_0 \leq N - p - n$, and it follows that λ_0 can take exactly $N - 2n - 2p + 1$ values. Once again, this is $2n$ values fewer than if the other complex were not present. Here it is important that in both cases it is the number n of waves in the *smaller* of the two complexes which appears. The total number of solutions is therefore

$$(N - 2n - 2p + 1)(N - 4n + 1).$$

It remains to consider the case $n = p$. In this case, for $\kappa = n - 1$, one of the partners $\mu = \kappa + 2$ is absent, which yielded a contribution $\psi_{\kappa,\mu} = \frac{1}{2}\pi$ previously, and similarly, for $\kappa = -(n-1)$, the partner $\mu = \kappa - 2$ is absent. In this case, therefore,

$$\sum_\kappa \sum_\mu \psi_{\kappa,\mu} = (2n - 1)\pi. \tag{43}$$

Moreover, there is now just one λ' such that $n \cot \frac{\pi\lambda'}{N} = p \cot \frac{\pi\lambda_0}{N}$, namely $\lambda' = \lambda_0$. This does not lead to a solution, however, since $f_\kappa = f_\mu$ whenever $\kappa = \mu$, and we know that the eigenfunction vanishes when two wave numbers are equal. At most, therefore, $Nk_1 = 2\pi(\lambda_0 - 1)$, and that yields

$$\begin{aligned} \lambda_1 &= \lambda_0 - \frac{1}{2} - n, \\ \lambda_2 &= \lambda_0 - \frac{1}{2} + n. \end{aligned}$$

Similarly, for $Nk_1 = 2\pi(\lambda_0 + 1)$,

$$\begin{aligned}\sum_\kappa \sum_\mu \psi_{\kappa,\mu} &= -(2n-1)\pi, \\ \lambda_1 &= \lambda_0 + \frac{1}{2} + n, \\ \lambda_2 &= \lambda_0 + \frac{1}{2} - n.\end{aligned}$$

λ_0 is in this case clearly a half-integer number. In the collection of values for λ_1, $2n$ numbers are again missing: $\lambda_0 - n + \frac{1}{2}, \ldots, \lambda_0 + n - \frac{1}{2}$, but in the collection of possible values for λ_0 only $2n-1$: λ_0 must be at least $2n - \frac{1}{2}$ ($\lambda_2 = n$), and can be at most $N - 2n + \frac{1}{2}$ ($\lambda_2 = N - n$), i.e. $N - 4n + 2$ values instead of the $N - 2n + 1$ possible values if there were only a single complex with n waves. Interchanging λ_1 and λ_2 does not change the solution, so the total number of solutions is

$$\frac{1}{2}(N - 4n + 2)(N - 4n + 1).$$

[The behaviour becomes perhaps even clearer if, for the moment, we normalise ψ differently: Let ψ' be defined in such a way that it agrees with ψ for large a, but remains continuous at $a = b$. Then, in the case of two complexes with n waves, $\sum_\kappa \sum_\mu \psi'_{\kappa,\mu}$ increases from zero to $(2n-1)2\pi$ when k_1 increases from $\frac{2\pi}{N}n$ to $\frac{2\pi}{N}(N-n)$ at constant k_2. Now, if

$$2\pi\lambda'_1 = Nk_1 - \sum_\kappa \sum_\mu \psi'_{\kappa,\mu}$$

then λ'_1 obviously takes all values n to $N - 3n + 1$, i.e. $N - 4n + 2$ values, whatever the value of λ_2. For λ_2, on the contrary, one more value has to be excluded, namely that which would lead to $k_1 = k_2$.]

We now consider the general case, in which there are q_n complexes, each with n waves, i.e. q_1 single waves with real wave numbers, q_2 pairs with conjugate complex wave numbers, etc. The constant λ_1 of the first complex with n waves would have the possible values $n, n+1, \ldots, N-n$, a total of $N - 2n + 1$ possible values, namely when no other wave complex were present. But, for every complex with $p > n$ waves, this collection of values is reduced, as we have seen, by $2n$ numbers, and for each complex with $p > n$ waves by $2p$, and finally, for the $q_n - 1$ complexes with n waves, by $2n - 1$. There remain

$$Q'_n = N - 2n + 1 - 2\sum_{p<n} p\, q_p - 2\sum_{p>n} n\, q_p - (2n-1)(q_n - 1)$$

possible values for λ_1. The constant λ_2 of the second complex of n waves, must in addition avoid k_2 being equal to k_1 and hence has one possibility less. For the last of the complexes of n waves, λ_{q_n} can take just

$$Q'_n - (q_n - 1) = Q_n + 1$$

values, where

$$Q_n(N, q_1, q_2, \dots) = N - 2\sum_{p<n} p\, q_p - 2\sum_{p\geq n} n\, q_p. \tag{44}$$

We finally have to take into account that interchanging λ's for different wave complexes with equal numbers n of waves does not lead to a new solution. The total number of solutions therefore becomes

$$z(N, q_1, q_2, \dots) = \prod_{n=1}^{\infty} \frac{(Q_n + q_n)\dots(Q_n + 1)}{q_n!} = \prod_n \binom{Q_n + q_n}{q_n}. \tag{45}$$

§8. We shall now prove that we have found the right number of solutions.

It is well-know that the number $z(r)$ of eigenvalues with given *total spin* $s = \frac{1}{2}N - r$ is equal to the number of eigenvalues with *total spin-component* of left-oriented spins $m = s$ minus those with $m = s + 1$, i.e.

$$z(N, r) = \binom{N}{r} - \binom{N}{r-1} = \frac{N - 2r + 1}{N - r + 1}\binom{N}{r}. \tag{46}$$

We must therefore have

$$\sum_{q_1, q_2, \dots} z(N, q_1, q_2, \dots) = z(N, r), \tag{47}$$

where the sum on the right-hand side runs over all values $q_1, q_2, \dots$ for which the total number of spin waves equals r, i.e.

$$q_1 + 2q_2 + 3q_3 + \dots = \sum n\, q_n = r.$$

In other words, we have to sum over all "partitions" of the number r; q_n indicates how often the summand n occurs in the partition.

We introduce the total number of spin complexes:

$$q = \sum_n q_n \tag{48}$$

and rewrite (44):

$$\begin{aligned} Q_n(N, q_1, q_2, \dots) &= N - 2q - 2\sum_{p<n}(p-1)q_p - 2\sum_{p\geq n}(n-1)q_p \\ &= Q_{n-1}(N - 2q, q_2, q_3, \dots). \end{aligned} \tag{49}$$

In particular,

$$Q_1(N, q_1, q_2, \dots) = N - 2q. \tag{49a}$$

Hence, using (45),

$$z(N, q_1, q_2, \dots) = \binom{N - 2q + q_1}{q_1} \cdot z(N - 2q, q_2, q_3, \dots). \tag{50}$$

In the right-hand side is, apart from the binomial coefficient, the number of solutions with q_2 single-spin waves, and in general q_n complexes of $n-1$ waves, in a chain of $N - 2q$ atoms. These solutions obviously contain a total

$$r' = \sum_n q_n(n-1) = r - q \tag{50-a}$$

of right-spins, arranged in

$$q' = \sum_{n=2}^{\infty} q_n = q - q_1 \tag{50-b}$$

wave complexes. We now also introduce a notation for the number of solutions in which r right-spins are organised in q wave complexes, irrespective of how many waves each complex contains:

$$z(N, r, q) = \sum_{\substack{q_1+q_2+q_3+\dots=q \\ q_1+2q_2+3q_3+\dots=r}} z(N, q_1, q_2, \dots). \tag{51}$$

Then we have, from (50), (50a) and (50b),

$$z(N, r, q) = \sum_{q_1=0}^{q-1} \binom{N - 2q + q_1}{q_1} z(N - 2q, r - q, q - q_1), \tag{52}$$

and

$$z(N, r) = \sum_{q=1}^{r} z(N, r, q). \tag{53}$$

From this point, we treat the problem using mathematical induction. We make the conjecture

$$z(N,r,q) = \frac{N-2r+1}{N-r+1}\binom{N-r+1}{q}\binom{r-1}{q-1}. \tag{54}$$

For $q=1$ this is certainly correct: We then have a single complex of r waves, whose wave number can take $N-2r+1$ values. It is also correct for $q=r$: then $q_1 = r$ and $q_n = 0$ for $n > 1$, and (54) is the same as (45). We now assume that (54) has been proven for $N-2q$, $r-q$, $q-q_1$, and have, according to (52),

$$\begin{aligned} z(N,r,q) &= \sum_{q_1=0}^{q-1}\binom{N-2q+q_1}{q_1}\binom{N-r-q+1}{q-q_1} \\ &\quad\times\binom{r-q-1}{q-q_1-1}\frac{N-2r+1}{N-r+1}. \end{aligned}$$

Now,

$$\binom{N-2q+q_1}{q_1} = \sum_{s=0}^{q_1}\binom{r-1}{s}\binom{N-2q+q_1+1-r}{q_1-s},$$

so

$$\begin{aligned} z(N,r,q) &= \sum_{q_1=0}^{q-1}\sum_{s=0}^{q_1}\frac{(N-r-q+1)!}{(q-q_1)!(N-r-2q+q_1+1)!}\frac{(N_r-2q+q_1+1)!}{(q_1-s)!(N_r-2q+s+1)!} \\ &\quad\times\frac{N-2r+1}{N_r+1}\binom{r-1}{s}\binom{r-q-1}{q-q_1-1} \\ &= \frac{N-2r+1}{N-r-q+1}\sum_{s=0}^{q-1}\binom{r-1}{s}\binom{N-r-q+1}{q-s} \\ &\quad\times\sum_{q=s}^{q-1}\binom{q-s}{q_1-s}\binom{r-q-1}{q-q_1-1} \\ &= \frac{N-2r+1}{N-r-q+1}\sum_{s}\frac{(r-1)!}{s!(r-s-1)!}\frac{(r-s-1)!}{(q-s-1)!(r-q)!} \\ &\quad\times\binom{N-r-q+1}{q-s} \\ &= \frac{N-2r+1}{N-r-q+1}\binom{r-1}{q-1}\sum_{s}\binom{q-1}{s}\binom{N-r-q+1}{q-s} \\ &= \frac{N-2r+1}{N-r-q+1}\binom{r-1}{q-1}\binom{N-r}{q}, \end{aligned}$$

which is identical to (54). Since (54) holds for $q = 1$ and for $q = 2$, $r = 2$, and trivially also for $q = 2$, $r = 1$, its validity can also be proved for $q = 2$, $r = 3$ or 4, then for $q = 2$ and larger values of r, finally for $q = 3$, 4, etc. Inserting (54) into (53) gives

$$\begin{aligned} z(N,r) &= \frac{N-2r+1}{N-r+1}\sum_{q=1}^{r}\binom{N-r+1}{q}\binom{r-1}{r-q} \\ &= \frac{N-2r+1}{N-r+1}\binom{N}{r}, \end{aligned}$$

which corresponds with the required number of solutions (46). *Our method therefore yields all solutions of the problem.*

In future work this method will be extended to spatial lattices, and the physical consequences *vis-a-vis* cohesion, ferromagnetism and conductivity will be derived.

Acknowledgement. I thank Prof. Fermi very much for the many lively discussions. I also thank the Rockefeller Foundation for providing a stipendium, which enabled my visit to Rome.

Rome, 13 June 1931.