

# On the Theory of Metals, I. Eigenvalues and Eigenfunctions of a Linear Chain of Atoms

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(Zeit. f. Physik **71**, 205 (1931))

A method is given whereby the zero-order eigenfunctions and first-order eigenvalues (in the sense of the London-Heitler approximation scheme) are calculated for a one-dimensional "metal" consisting of a linear chain of a very large number of atoms, each of which has a single  $s$ -electron with spin, outside closed shells. In addition to the spin waves of Bloch, bound states are found, in which parallel spins are predominantly on nearest neighbor atoms; these features may be important for the theory of ferromagnetism.

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## I. INTRODUCTION

Until now, the theory of metals has for some time been limited to the investigation of the motion of individual conduction electrons in the potential field of the metal atoms (Sommerfeld, Bloch). The interaction of electrons with one another has been ignored, at least insofar as the electronic-interaction potentials are concerned. Although this procedure has been very fruitful in problems of metallic conductivity (with the exception of superconductivity), it did not allow for a deeper penetration into the problem of ferromagnetism [1] and for example, it rendered the calculation of the cohesive forces in metals a completely hopeless undertaking: exchange forces among the conduction electrons dominate first order perturbation theory and have the same order of magnitude as the zero-point energy of the electron gas (the energy in zeroth-order perturbation theory). Accordingly, one estimates that the second-order approximation will again be of the same order of magnitude, and so on. Under such circumstances, one should be skeptical of an approximation in which the motional energy of the electrons (kinetic zero-point energy) is considered to be overwhelmingly more important than their interaction energy (exchange energy).

It is for such reasons that Slater [2] and Bloch [3] have recently tried to approximate the problem from another angle, that is assuming the atomic structures to be given and their interactions to be the perturbation, in accordance with the London-Heitler approximation for molecules. Slater was mainly interested in the cohesive energy of non-ferromagnetic materials, in which the London-Heitler exchange integral is generally negative [4]<sup>1</sup>, and gave an interesting method for the approximate calculation of the ground state energy of such metals when the total spin vanishes. In the case of ferro-

magnetism, Bloch calculated approximately the leading terms in the opposite case  $J > 0$ <sup>2</sup> in a systematic fashion, but obtained too many eigenvalues by his method. It is the aim of the present work first, to give a procedure for the case of a linear chain of atoms, which allows the calculation of every eigenvalue of this one-dimensional crystal to arbitrary within the context of the first approximation of the London-Heitler method, such that the problem will be at exactly the same stage as the hydrogen molecule  $H_2$  in the London and Heitler work. And in addition, to obtain other types of solutions differing from the (somewhat modified) Bloch [3] solutions, ensuring that the total number of eigenvalues turns out exactly correct.

## II. FORMULATION

Our problem can be stated as follows: Given a linear chain composed of a large number ( $N$ ) of like atoms where each atom has a single valence electron in an  $s$ -orbit outside closed shells occupying a known atomic eigenfunction, what are the zeroth-order eigenfunctions and first-order eigenvalues of the entire system when the interaction among the individual atoms is taken into account?

As long as one neglects the interaction energies, there are two states of equal energy for each atom—the spin of the valence electron can point either right or left. The energy eigenvalue of the chain is therefore  $2^N$ -fold degenerate in zeroth approximation. Each of these states of the chain can be specified by enumerating the atoms which carry a right-handed spin; assume this to be the case for atoms  $m_1, m_2, \dots, m_r$ . The corresponding totally antisymmetric eigenfunction of the chain is

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<sup>1</sup>Here,  $J < 0$  implies "antiferromagnetic" couplings

<sup>2</sup>Here,  $J > 0$  implies "ferromagnetic" couplings

$\varphi(m_1, m_2, \dots, m_r)$ . The correct zeroth-order eigenfunctions therefore assume the form

$$\Psi = \sum_{m_1, m_2, \dots, m_r} a(m_1, m_2, \dots, m_r) \varphi(m_1, m_2, \dots, m_r)$$

where each of the integers  $m_1, m_2, \dots, m_r$  runs from 1 to  $N$ . We specialize to  $m_1 < m_2 < \dots < m_r$ .

One calculates matrix elements of the interaction energy using these states, each specified by its spin distribution  $m_1, m_2, \dots, m_r$ , obtaining: [3]

*Diagonal Elements:* If in the spin distribution  $m_1, m_2, \dots, m_r$  these are  $N'$  nearest neighbor pairs of parallel spins, then

$$W_{m_1, m_2, \dots, m_r} = E_0 - N'J.$$

$E_0$  is the electrostatic interaction energy of the atoms are neglected, as they fall off exponentially with distance.

*Nondiagonal Elements* occur between any two states which differ merely by a single perturbation of a pair of adjacent antiparallel spins as, for example, between  $m_1, \dots, m_i, \dots, m_r$  (where we suppose  $m_i + 1$  to be a left-handed spin and therefore missing from the enumeration) and  $m_1, \dots, m_i + 1, \dots, m_r$ , (with  $m_i$  missing). All such off-diagonal matrix elements have a value  $-J$ .

With the aid of the interaction matrix elements, one obtains the following equations among the coefficients  $a(m_1, m_2, \dots, m_r)$  of the eigenstate  $\Psi$  which we are seeking:

$$2\varepsilon a(m_1, \dots, m_r) + \sum \{a(m'_1, \dots, m'_r) - a(m_1, \dots, m_r)\} = 0 \quad (1)$$

Here,

$$2\varepsilon J = \varepsilon - E_0 + NJ \quad (2)$$

and  $\varepsilon$  is the total first-order perturbation energy. The summation is over all sets  $m'_1, m'_2, \dots, m'_r$  which differ from  $m_1, m_2, \dots, m_r$  by a single permutation of nearest-neighbor antiparallel spins.<sup>3</sup>

In addition to Eqs.(1), the  $a$ 's must satisfy periodic boundary conditions:

$$a(m_1, \dots, m_i, \dots, m_r) = a(m_1, \dots, m_i + N, \dots, m_r) \quad (3)$$

### III. REAL SOLUTIONS

For  $r = 1$  the solution of (1) is

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

For  $r = 2$ , two cases are to be distinguished: either the two right-handed spins are separated, in which case

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

with  $m_2 \neq m_1 + 1$ , or else they are adjacent, and:

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

The first set of equations are rigorously solved by an ansatz,

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

in which  $c_1, c_2, f_1, f_2$  are as yet undetermined by all this.

The second set can be satisfied by selecting  $c_1$  and  $c_2$  so as to satisfy

$$0 = a(m_1, m_1) + a(m_1 + 1, m_1 + 1) - 2a(m_1, m_1 + 1). \quad (6)$$

Here,  $a(m_1, m_1)$  has no physical meaning but, rather, is to be defined by (5). Obviously, by adding (6) to (4b) we bring it to the form (4a), and we have already satisfied equations of this type. Inserting (5) into (6) yields:

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

$$\frac{c_1}{c_2} = -\frac{\cos \frac{f_1 + f_2}{2} - e^{i(\frac{f_1 - f_2}{2})}}{\cos \frac{f_1 + f_2}{2} - e^{-i(\frac{f_1 - f_2}{2})}} = \frac{\sin \frac{f_1 - f_2}{2} + ic_{12}}{\sin \frac{f_1 - f_2}{2} - ic_{12}}$$

with  $c_{12} = \cos \frac{f_1 + f_2}{2} - \cos \frac{f_1 - f_2}{2} [= -2 \sin \frac{f_1}{2} \sin \frac{f_2}{2}]$  [Editor's note:  $|c_1/c_2| = 1$ , therefore we just seek a phase factor.] Set  $c_1 = e^{i\frac{\varphi}{2}}$ ,  $c_2 = e^{-i\frac{\varphi}{2}}$ , so that

$$\begin{aligned} \cot \frac{\varphi}{2} &= \frac{\sin \frac{f_1 - f_2}{2}}{c_{12}}, \\ 2 \cot \frac{\varphi}{2} &= \cot \frac{f_1}{2} - \cot \frac{f_2}{2}. \end{aligned} \quad (8)$$

Thus, one obtains

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

Additionally, it is assumed that  $m_1$  and  $m_2$  lie in the fundamental period of the chain, i.e.,  $1 \leq m_1 < m_2 \leq N$ . Periodic boundary conditions require:

$$a(m_1, m_2) = a(m_2, m_1 + N). \quad (10)$$

<sup>3</sup>Eq.(1) is more extensively derived by Bloch in Eq.(5) of Ref.3, where he labels atoms  $f_i$  instead of  $m_i$ , and instead of  $2\varepsilon J$ , simply writes as  $\varepsilon$ .

[The notation  $a(m_2, m_1 + N)$  is explained by our convention of listing the  $m_i$  in the order of increasing magnitude, see above.] Inserting (9) into (10):

$$e^{i(f_1 m_1 + f_2 m_2 + \frac{\varphi}{2})} + e^{i(f_2 m_1 + f_1 m_2 - \frac{\varphi}{2})} \\ = e^{i(f_1 m_2 + f_2(m_1 + N) + \frac{\varphi}{2})} + e^{i(f_2 m_2 + f_1(m_1 + N) - \frac{\varphi}{2})}.$$

As these must hold for all  $m_1$  and  $m_2$ , the first term on the left must be equal to the second term on the right, as they have the same dependence on  $m_1$  and  $m_2$ , and conversely, so that

$$Nf_1 - \varphi = 2\pi\lambda_1, Nf_2 + \varphi = 2\pi\lambda_2, \quad (11)$$

and  $\lambda_1, \lambda_2 = 0, 1, 2, \dots, N - 1$ . Although, individually, the  $f_1$  and  $f_2$  do not have the usual form  $\frac{2\pi\lambda}{N}$ , their sum,

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

is a true constant of the motion of the problem; the coefficient  $a(m_1, m_2)$  is multiplied by  $e^{ik}$  if both the right-handed spins are displaced by one atomic position to the right, a translation which obviously does not affect any physical properties [by translation invariance].

We now discuss the behavior of the phase  $\varphi$  as a function of  $f_1$  and  $f_2$ , for which we specify that

$$-\pi \leq \varphi \leq \pi. \quad (13)$$

If one interchanges  $f_1$  and  $f_2$ , then clearly  $\varphi$  changes sign and the coefficients remain unchanged, according to (9). If  $f_2$  is held fixed and  $f_1$  is allowed to increase from zero, then  $\cot \frac{\varphi}{2}$  falls from  $+\infty$  to smaller positive values, finally reaching zero for  $f_1 = f_2$ ; thus,  $\varphi$  ranges from 0 to  $\pi$ . If  $f_1$  becomes slightly greater than  $f_2$ ,  $\varphi$  jumps from  $\pi$  to  $-\pi$ , gradually increasing back to zero as  $f_1$  increases to  $2\pi$ . If  $f_1 = f_2$ , then either

$$\varphi = +\pi, \lambda_1 = \lambda_2 - 1 = \frac{Nf_1}{2\pi} - \frac{1}{2},$$

or

$$\varphi = -\pi, \lambda_1 = \lambda_2 + 1 = \frac{Nf_1}{2\pi} + \frac{1}{2}.$$

In either instance, according to (9) for all  $m_1, m_2$ ,  $a(m_1, m_2)$  becomes

$$a(m_1, m_2) = e^{if_1(m_1 + m_2)}(e^{i\frac{\varphi}{2}} + e^{-i\frac{\varphi}{2}}) \equiv 0.$$

This means that  $f_1 = f_2$ <sup>4</sup> does not lead to a meaningful solution of the problem, and if  $\lambda_2$  is specified,  $\lambda_1$  can take on only the values

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

As  $f_1, f_2$  and  $f_2, f_1$  yield the same eigenfunction, we can specify  $f_1 < f_2$  without loss of generality. Thus, for fixed  $\lambda_2$ , there are  $\lambda_2 - 1$  solutions  $\lambda_1 = 0, 1, \dots, \lambda_2 - 2$  and  $\lambda_2$  goes from 2 to  $N - 1$ , so that the total number becomes:

$$\sum_{\lambda_2=2}^{N-1} (\lambda_2 - 1) = \binom{N-1}{2} \equiv \frac{(N-1)!}{2!(N-3)!}$$

a binomial coefficient. Clearly, there must be as many solutions as there are distinct configurations for  $m_1$  and  $m_2$ , namely  $\binom{N}{2} = \frac{N!}{2!(N-2)!}$ . So in fact the foregoing exact analysis yields an *insufficient number* of solutions, whereas Bloch [3] believed that the method yields too many, namely  $\binom{N+1}{2} = \frac{(N+1)!}{2!(N-1)!}$ .

#### IV. ADDITIONAL IMAGINARY SOLUTIONS

There must exist  $N - 1$  additional solutions. These are obtained by allowing the wave numbers  $f_1$  and  $f_2$  to take on complex-conjugate values. In fact we shall find that for each, arbitrary, value of  $k = f_1 + f_2$  there is found precisely one pair of complex conjugate solutions to Eqs.(8) and (11)<sup>5</sup>. Let

$$f_1 = u + iv, \quad (14) \\ f_2 = u - iv,$$

then

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

By (11),

$$N(f_1 - f_2) = 2Niv = 2\pi(\lambda_1 - \lambda_2) + 2\varphi, \\ \varphi = \psi + i\chi, \\ \psi = \pi(\lambda_2 - \lambda_1), \\ \chi = Nv. \quad (16)$$

If  $v$  is finite, then  $\chi$  must be very large, such that

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

<sup>4</sup> $\lambda_1 = \lambda_2 \pm 1$

<sup>5</sup>the "bound-state"

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

In *first* approximation, the following holds:

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

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

$$e^{-v} = \cos u \quad (18)$$

and

$$\begin{aligned} \varepsilon &= 2 - \cos(u + iv) - \cos(u - iv) \\ &= 2 - 2 \cos u \cosh v = 2 - \cos u \left( \cos u + \frac{1}{\cos u} \right), \\ \varepsilon &= \sin^2 u = \frac{1}{2}(1 - \cos 2u). \end{aligned} \quad (19)$$

Clearly,  $\cos u$  has to be  $\geq 0$ , that is  $-\frac{\pi}{2} \leq u \leq \frac{\pi}{2}$ . If then  $k = 2u + 2n\pi$  ( $n$  an integer) is between 0 and  $\pi$ , then

$$u = \frac{k}{2},$$

if between  $\pi$  and  $2\pi$ , then

$$u = \frac{k}{2} + \pi.$$

In a *second* approximation we set

$$v = v_0 + \varepsilon, \quad (20)$$

where  $v_0$  is value obtained in the first approximation. Then,

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

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<sup>6</sup>In fact, this occurs already for  $u < \frac{2}{\sqrt{N}}$ , despite that in the second approximation  $v$  is positive, because higher approximations push it down to negative values.

$$\varepsilon = (\tan^2 u)e^{-\chi+i\psi}.$$

As  $\varepsilon$  is in general very small,  $Nv_0$  can be written for  $\chi$ .  $\psi$  is now adjusted according to the prescribed value of  $k$ :

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

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

Likewise, for  $\lambda \geq \frac{N}{2}$ ,  $N + \lambda$  even:

$$\lambda_1 = \lambda_2 = \frac{N + \lambda}{2}, \psi = 0.$$

If either  $\lambda$  or  $N + \lambda$  is odd, then we must write:

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

From this,

$$\varepsilon = \pm \tan^2 u e^{-Nv_0}. \quad (21)$$

For even  $\lambda$  (or  $N + \lambda$ ),  $v > v_0$ . If in the next approximation  $v_0$  is replaced by  $v$  then resulting  $\varepsilon$  is smaller than that of the second approximation. The procedure for the determination of  $v$  always converges, indeed very rapidly. On the other hand, if a negative sign be chosen (odd  $\lambda$  or  $N + \lambda$ ) then  $v < v_0$  and absolute value of  $\varepsilon$  increases in higher approximations. This makes no difference so long as  $v_0$  is finite, as then the correction to  $\varepsilon$  is infinitesimal. But if  $u$  is small and therefore  $\cos u \approx 1$ , then  $v_0$  is also small, and to sufficient accuracy

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

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

$$\varepsilon = -u^2 e^{-Nv_0}$$

is larger than  $v_0$  in absolute value so long as  $Nv_0 < \log 2 \approx 0.7$ ,  $u^2 < \frac{1.4}{N}$ . For  $u < \sqrt{\frac{1.4}{N}}$  and odd  $\lambda$ , then  $v_1 = v_0 + \varepsilon$  will be negative, the process diverges, and no solution with two complex conjugate wave numbers can be found. <sup>6</sup>

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In its place, there occurs an additional solution with two real wave numbers. We again consider  $k$  as given and  $f_2 = k - f_1$ . Earlier in the discussions of real solutions it was tacitly assumed that with increasing  $f_1$ ,  $F = Nf_1 - \varphi$

increased monotonically. This might seem obvious, insofar as  $f_1$  is multiplied by a very large factor  $N$  and  $\varphi$  is  $o(1)$ . Nevertheless, this assumption is invalid at small  $k$ . Looking at (8) in some greater detail, we obtain

$$\frac{dF}{df_1} = N - 2\frac{A}{D},$$

where

$$A \equiv \frac{1}{4 \sin^2 \frac{f_1}{2}} + \frac{1}{4 \sin^2 \frac{k-f_1}{2}}$$

and

$$D \equiv 1 + \left[ \frac{1}{2} \cot \frac{f_1}{2} - \frac{1}{2} \cot \frac{k-f_1}{2} \right]^2;$$

setting  $f_1 = f_2 = \frac{k}{2}$ , then clearly

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

is positive only so long as  $\sin \frac{f_1}{2} > \frac{1}{\sqrt{N}}$ . For  $k < 4 \sin^{-1}(\frac{1}{\sqrt{N}}) \approx \frac{4}{\sqrt{N}}$  the increase of  $F = Nf_1 - \varphi$  as function of  $f_1$  is broken off by a decrease in the vicinity of  $f_1 = \frac{k}{2}$ . If  $\frac{Nk}{2\pi} = \lambda$  is odd, then

$$\frac{Nk}{2} - \pi = 2\pi\lambda_1 = 2\pi\frac{\lambda-1}{2}$$

where  $\lambda_1$  is an integer, and for  $\lambda_1 = \frac{\lambda-1}{2}$ ,  $\lambda_2 = \frac{\lambda+1}{2}$ , there are two<sup>7</sup> solutions of the system of equations (8) and (11): besides  $f_1 = f_2$ ,  $\varphi = \pi$ , there exists a solution  $f_1 < f_2$ ,  $\varphi \neq \pi$ , for which the coefficients (9) remain finite in contrast to the first solution.

To actually find this solution, we put  $f_1 = f - 2\frac{\varepsilon}{N}$  and throughout and use  $\sin f = f$ ,  $\cos f = 1$ ,  $\cot f = \frac{1}{f}$ , valid for small  $f$ . Then,

$$2 \cot \frac{\varphi}{2} = \frac{2}{f - 2\frac{\varepsilon}{N}} - \frac{2}{f + 2\frac{\varepsilon}{N}} = \frac{8\varepsilon}{Nf^2} \quad (8a)$$

$$2\varphi = 2\pi(\lambda_2 - \lambda_1) - N(f_2 - f_1) = 2\pi - 4\varepsilon \quad (11a)$$

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

$$\frac{\tan \varepsilon}{\varepsilon} = \frac{4}{Nf^2}. \quad (22)$$

<sup>7</sup>One can show that  $F$  can assume no other integer value more than once (for odd  $\lambda$ ) and none at all for even  $\lambda$ .

<sup>8</sup>The solution  $\lambda_1 = N-1$ ,  $\lambda_2 = N$  has, in fact, already been counted once, in the form  $\lambda_2 = 0$ ,  $\lambda_1 = N-1$ .

From this,  $\varepsilon$  is determined,  $\varepsilon$  is  $< \frac{\pi}{2}$ , therefore  $\varphi > 0$  and  $Nf_1 > 2\pi\lambda_1$ .

With this, we have determined an additional solution, with real or complex wave number, at each value of  $\lambda$ . The largest allowed value of  $\lambda$  is obviously  $N-2$  with  $\lambda_1 = \lambda_2 = N-1$ ; for  $\lambda = N-1$  on the other hand,  $\lambda_2 = N$ , outside the permissible interval<sup>8</sup>. Thus, we find  $N-1$  solutions  $\lambda = 0, 1, 2, \dots, N-2$ , precisely the required number.

According to Eqs.(9), (12), (16a), the coefficients  $a(m_1, m_2)$  of our complex solutions are

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

$$a(m_1, m_2) = e^{iu(m_1+m_2)} \left\{ \begin{array}{l} \cosh \\ \sinh \end{array} \right\} v \left( \frac{N}{2} - (m_2 - m_1) \right) \quad (23)$$

with  $\cosh$  or  $\sinh$  applying according to whether  $\lambda$  (or  $N+\lambda$  for  $\lambda > \frac{N}{2}$ ) is even or odd. For our solutions it is most probable that both right-handed spins lie as close together as possible, as the probability  $|a(m_1, m_2)|^2$  falls off exponentially with distance  $m_2 - m_1$ . The extreme case occurs for the solution with  $\lambda = \frac{N}{2}$ ,  $u = \frac{\pi}{2}$  and  $v = \infty$ . Here, after appropriate normalization,

$$a(m_1, m_2) = \left\{ \begin{array}{ll} 0 & \text{for } m_2 \neq m_1 + 1 \\ (-1)^{m_1} & \text{for } m_2 = m_1 + 1 \end{array} \right. ,$$

and both spins are always precisely adjacent.

Every eigenvalue  $\varepsilon$  for a solution with two complex conjugate wave numbers is *smaller* than any eigenvalue with the same total wave number  $k$  and real wave numbers, as we shall now show. According to (2) then, the corresponding energy  $e$  in the first approximation is *lower* than all the solutions with real wave numbers if the exchange integral  $J$  is positive (for ferromagnetism) or higher, if  $J$  is negative (the usual case).

For the complex solution we have, specifically,

$$\varepsilon_k = \sin^2 u, \quad (19)$$

whereas for the real,

$$\varepsilon_r = 1 - \cos f_1 + 1 - \cos(k - f_1), \quad (5)$$

(5) reaches its minimum for

$$f_1 = \left\{ \begin{array}{ll} \frac{k}{2} & \text{for } 0 \leq k \leq \pi \\ \frac{k}{2} + \pi & \text{for } \pi \leq k \leq 2\pi \end{array} \right. ,$$

that is, generally for  $f_1 = f_2 = u$ . The minimum is

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

so that

$$\frac{\varepsilon_k}{\varepsilon_{min}} = \frac{1 + \cos u}{2} \leq 1, \quad (24)$$

where the equal sign applies only at  $u = 0$ <sup>9</sup>. QED.

## V. GENERAL CASE

We turn now to the general case of  $r$  right-handed spins. Eqs.(1) again fall into two types: If none of the  $r$  designated spins  $m_1, \dots, m_r$  are adjacent, then

$$\begin{aligned} -2\varepsilon a(m_1, \dots, m_i, \dots, m_r) &= \sum_{r=1}^r [a(m_1, \dots, m_i+1, \dots, m_r) \\ &+ a(m_1, \dots, m_i-1, \dots, m_r) - 2a(m_1, \dots, m_i, \dots, m_r)]. \end{aligned} \quad (24a)$$

If instead, two are adjacent, say  $m_{k+1} = m_k + 1$ , then,

$$\begin{aligned} -2\varepsilon a(m_1, \dots, m_i, \dots, m_k, m_k+1, \dots, m_r) \\ = a(\dots, m_k-1, m_k+1, \dots) + a(\dots, m_k, m_k+2, \dots) \\ - 2a(\dots, m_k, m_k+1, \dots) + \sum_{i \neq k, k+1}^r [a(\dots, m_i+1, \dots) \\ + a(\dots, m_i-1, \dots) - 2a(\dots, m_i, \dots)] \end{aligned} \quad (24b)$$

and analogously for any larger number of adjacent right-handed spins.

We next suppose<sup>10</sup>

$$a(m_1, \dots, m_i, \dots, m_r) = \sum_{P=1}^{r!} e^{i[\sum_{k=1}^r f_{P_k} m_k + \frac{1}{2} \sum \varphi_{P_k, P_n}]} \quad (25)$$

$$\varepsilon = \sum_{k=1}^r (1 - \cos f_k). \quad (26)$$

$P$  is any permutation of the  $r$  numbers  $1, 2, \dots, r$ , and  $P_k$  is the number which replaces  $k$  under this permutation. The ansatz satisfies the first set of equations (24a)

by inspection. The remaining equations are satisfied by requiring that

$$\begin{aligned} 2a(\dots, m_k, m_k+1, \dots) \\ = a(\dots, m_k, m_k, \dots) + a(\dots, m_k+1, m_k+1, \dots) \end{aligned} \quad (27)$$

in which the<sup>11</sup> amplitudes on the right are to be *defined* according to (25). Eq.(27) must hold for any arbitrary set of  $m_1, m_2, \dots, m_r$  of which an arbitrary number can be nearest-neighbors, provided only  $m_1 < m_2 < \dots < m_r$ . All the relations (24b) are simultaneously satisfied by this device, including cases in which the  $m_1, m_2, \dots, m_r$  involve more than one pair of adjacent parallel spins; all equations are reduced to the type (24a), which have already been solved. Eq.(27) itself is satisfied by requiring the phase  $\varphi$  to satisfy the relations,

$$2 \cot \frac{\varphi_{kn}}{2} = \cot \frac{f_k}{2} - \cot \frac{f_n}{2}; \quad (28)$$

$$-\pi \leq \varphi_{kn} \leq \pi.$$

There remain the periodic boundary conditions,

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

$$\begin{aligned} \sum_P e^{i[\sum_{k=1}^r f_{P_k} m_k + \frac{1}{2} \sum \varphi_{P_k, P_n}]} \\ = \sum_{P'} e^{i[\sum_{k=2}^r f_{P'_k} m_k + f_{P'_1} (m_1 + N) + \frac{1}{2} \sum_{k < n} \varphi_{P'_k, P'_n}]} \end{aligned}$$

This holds for all  $m_1, m_2, \dots, m_r$ ; therefore terms on the left-hand and right-hand sides of the equation which have the same dependence on  $m_k$  must be precisely equal. For example, consider a term  $P$  on the left and  $P''$  on the right, with  $P''$  defined by

$$P''_{k-1} = P_k (k = 2, \dots, r), P''_r = P_1.$$

These results

$$\begin{aligned} N f_{P''_r} + \frac{1}{2} \sum_{k < n} \varphi_{P''_k, P''_n} - \frac{1}{2} \sum_{k < n} \varphi_{P_k, P_n} = 2\pi\lambda \\ = N f_{P_1} + \frac{1}{2} \sum_{k < n \leq r-1} \varphi_{P_{k+1}, P_{n+1}} + \frac{1}{2} \sum_{k=1}^{r-1} \varphi_{P_{k+1}, P_1} \end{aligned}$$

<sup>9</sup>As  $f_1$  is never exactly equal to  $f_2$  (cf. Sec.III), in fact the inequality always applies.

<sup>10</sup>"Bethe ansatz"

<sup>11</sup>"unphysical"

$$\begin{aligned}
& -\frac{1}{2} \sum_{2 < k \leq n} \varphi_{P_k, P_n} - \frac{1}{2} \sum_2^r \varphi_{P_1, P_k} \\
& = N f_{P_1} - \sum_{k=2}^r \varphi_{P_1, P_k},
\end{aligned}$$

making use of  $\varphi_{kn} = -\varphi_{nk}$ . Since this relation holds for every  $P$ , it follows that

$$N f_i = 2\pi \lambda_i + \sum_{k \neq i} \varphi_{ik} \quad (29)$$

for all  $i = 1, \dots, r$ .

In complete analogy with Sec.III, one further can show that two  $f_i$ 's can never coincide, otherwise all the coefficients vanish, and therefore for real  $f_i$  two succeeding  $\lambda_i$ 's must differ by at least 2. The number of solutions with real  $f$ 's is thus

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

far fewer than

$$\binom{N}{r},$$

the number of solutions we seek.

## VI. COMPLEX SOLUTIONS

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

$$N f_k = 2\pi \lambda_k + \sum_{n \neq k} \varphi_{kn}$$

that at least one of the  $\varphi_{kn}$ 's has to have a very large imaginary part of  $O(N)$ . That means in first approximation (cf. Sec.IV)

$$2 \cot \frac{\varphi_{kn}}{2} = \cot \frac{f_k}{2} - \cot \frac{f_n}{2} = -2i.$$

That is, there must be an  $f_n$  such that the real part of  $\cot \frac{f_n}{2}$  must agree with that of  $\cot \frac{f_k}{2}$ , while their imaginary parts differ by 2 (to  $O(e^{-N})$ ). One is led to the following solution, which we shall denote a *wavecomplex*<sup>12</sup>:  $n$  wave numbers are defined by the equations:

$$\cot \frac{f_k}{2} = a - i\kappa; \kappa = -(n-1), -(n-3), \dots, (n-3), (n-1) \quad (30)$$

in which  $a$  is a constant for all  $n$  wave numbers. Clearly,

$$\varphi_{\kappa, \kappa \pm 2} = \psi - (\pm i)\infty$$

where the remaining  $\varphi$ 's have finite imaginary parts.  $\psi$  remains undetermined. Applying (15) one obtains

$$\frac{\sin u_\kappa}{\cosh v_\kappa - \cos u_\kappa} = a,$$

$$\frac{\sinh v_\kappa}{\cosh v_\kappa - \cos u_\kappa} = \kappa,$$

for which the solutions are

$$u_\kappa = \tan^{-1} \frac{2a}{a^2 + \kappa^2 - 1} = \cot^{-1} \frac{a}{\kappa + 1} - \cot^{-1} \frac{a}{\kappa - 1}, \quad (31)$$

$$\tanh v_\kappa = \frac{2\kappa}{a^2 + \kappa^2 + 1},$$

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

and  $\sin u$  has therefore the sign of  $a$ .

We assert that  $a$  can be expressed using the total wave number of our wavecomplex,

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

which, in simplest form, is

$$a = n \cot \frac{k}{2}. \quad (34)$$

For  $n = 1$  this is evident, for  $n = 2$  it follows by inserting the solution obtained earlier (Eq.(18), Sec.IV)

$$e^{-v} = \cos u, u = \frac{k}{2} \quad (\text{or } \frac{k}{2} + \pi),$$

$$\begin{aligned}
a &= \frac{\sin u}{\cosh v - \cos u} = \frac{\sin u}{\frac{1}{\cos u} + \cos u - \cos u} \\
&= 2 \cot u = 2 \cot \frac{k}{2}.
\end{aligned}$$

On the other hand, at fixed  $a$ , the wave numbers for a complex of  $n$  waves are exactly the same as for a complex

<sup>12</sup>a many-spin bound state, i.e., a "soliton"

of only  $n-2$  waves, there are only two new wave numbers  $u_{n-1} = u_{-(n-1)}$  to be added, so that

$$\frac{k_n}{2} = \frac{k_{n-2}}{2} + u_{n-1}. \quad (33a)$$

Now taking (34) for  $n-2$  as proven, then

$$\frac{k_n}{2} = \cot^{-1} \frac{a}{n-2} + \cot^{-1} \frac{a}{n} - \cot^{-1} \frac{a}{n-2} = \cot^{-1} \frac{a}{n}.$$

We further assert that our wavecomplex has eigenvalue

$$\varepsilon_n = \frac{1 - \cos k}{n}. \quad (35)$$

This is also evident for  $n=1$ , and for  $n=2$  proved in (19). In general,

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

using (31), (32). We now assume (35) to be valid for  $n-2$  and use (34), from which it follows that

$$\begin{aligned} \frac{\varepsilon_n}{2} &= \frac{1}{(n-2)(1 + \frac{a^2}{(n-2)^2})} + 2 \frac{a^2 - n(n-2)}{(a^2 + n^2)(a^2 + (n-2)^2)} \\ &= \frac{(n-2)(a^2 + n^2) + 2(a^2 - n(n-2))}{(a^2 + n^2)(a^2 + (n-2)^2)} \\ &= \frac{n}{a^2 + n^2} = \frac{1 - \cos k}{2n} \end{aligned}$$

Finally, by analogy with Sec.IV, we establish the following: if the number of right-handed spins  $r$  and the total wave number  $k$  of all spin waves is given, then one obtains the smallest eigenvalue  $\varepsilon$  when one combines all  $r$  spin waves into a single wavecomplex of eigenvalue

$$\varepsilon_r = \frac{1 - \cos k}{r}.$$

For if one has *two* wavecomplexes with  $n$  and  $p = r - n$  waves, then

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

The minimum of this expression is at

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

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

and is

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

Certainly,

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

as immediately seen by squaring both sides. From this it follows directly that

$$\varepsilon_r < \varepsilon_{min}. \quad (36)$$

If the spin waves are composed of more than two wavecomplexes, naturally  $\varepsilon$  is still larger. The state of lowest energy for  $r$  right-handed spins is then, for  $J > 0$  (ferromagnetic case), a single wavecomplex of  $r$  spins; or, if  $J < 0$  (the more usual case),  $r$  individual waves with real wave numbers. In the latter instance, of course, the lowest energy state has not yet been fixed by this expedient.

It is easy to compute the second approximation for the wave numbers in a wavecomplex, by using the  $u$  and  $v$  of formulas (31), (32), altering them slightly in order to satisfy the actual periodic boundary conditions (29). The solution proceeds analogously to Sec.IV; one finds that in general for finite  $k$  one solution in the immediate vicinity of (31), (32) is allowed, while for small  $k$  of  $O(\frac{1}{\sqrt{N}})$ , the nature of the solution changes if  $\frac{Nk}{2\pi} = \lambda$  is indivisible by  $n$ . Instead of a complex of three spin waves there would occur, for example, a pair of conjugate complex waves as were already analyzed in Sec.IV for even  $\lambda$ , together with a single wave of almost the same, but real, wave number. The number of solutions is unaffected by this change of appearance. There is one solution for  $\lambda = 0, 1, 2, \dots, N - n$ ; the last value corresponds to  $\lambda_{-(n-1)} = \lambda_{-(n-3)} = \dots = \lambda_{n-1} = N - 1$ . For  $\lambda > N - n$ , one or more  $\lambda_\kappa$  would be  $N$ , which is not allowed.

From now on we shall also exclude  $\lambda_i = 0$  in general. We immediately gain in symmetry from this, and automatically distinguish those solutions for which the left-handed component of total spin  $M = \frac{N}{2} - r = S_{tot}$ , the total spin, from all those others with the same value of  $M$  which belong to a higher value of  $S_{tot}$ . The latter are just those states in which one or more of the  $r$  wave numbers are zero. After eliminating them, there remain only  $N - 2n + 1$  wavecomplex solutions of  $n$  spin waves:  $\lambda = n, n + 1, \dots, N - n$ .

## VII. THE NUMBER OF SOLUTIONS

We assume that *two* complexes of  $p$  ( $> n$ ) spin waves are available, and ask about the number of solutions that can be obtained by means of the ansatz. This leads us to discuss the phases  $\varphi$ . If the wave numbers in the first complex are given by

$$\cot \frac{f_\kappa}{2} = a - i\kappa, \quad \kappa = -(n-1), (n-3), \dots, n-1$$

$$a = n \cot \frac{k_1}{2}, \quad k_1 = \sum_\kappa f_\kappa \quad (37a)$$

and in the second by

$$\cot \frac{f_\mu}{2} = b - i\mu, \quad \mu = -(p-1), (p-3), \dots, p-1$$

$$b = p \cot \frac{k_2}{2}, \quad k_2 = \sum_\mu f_\mu \quad (37b)$$

then by (28), (29), (31)

$$Nk_1 = 2\pi\lambda_1 + \sum_\kappa \sum_\mu \varphi_{\kappa\mu},$$

$$Nk_2 = 2\pi\lambda_2 - \sum_\kappa \sum_\mu \varphi_{\kappa\mu},$$

$$\cot \frac{\varphi_{\kappa\mu}}{2} = \cot \left( \frac{\psi_{\kappa\mu}}{2} + i \frac{\chi_{\kappa\mu}}{2} \right) = \frac{a-b}{2} - i \frac{\kappa-\mu}{2},$$

$$\tan \psi_{\kappa\mu} = \frac{a-b}{\left(\frac{a-b}{2}\right)^2 + \left(\frac{\kappa-\mu}{2}\right)^2 - 1}. \quad (38)$$

The sign of  $\psi_{\kappa\mu} = \text{sign of } a-b$ , and  $\sum_\kappa \sum_\mu \chi_{\kappa\mu} = 0$ , because the  $f_\kappa$  and  $f_\mu$  come in ordered complex conjugate pairs.

The  $\psi_{\kappa\mu}$  are zero if  $k_1$  is very small,  $a$  very large, and then with increasing  $k_1$  they become positive as long as  $a > b$ . We are interested most of all in their for the case where  $a$  approaches  $b$  very closely and ultimately becomes smaller than  $b$ , in order to determine the number of forbidden integers  $\lambda_1, \lambda_2$ . For this we fix <sup>13</sup>  $\lambda_0 = \frac{Nk_2}{2\pi}$  and define  $\lambda'$  through

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

For  $Nk_1 = 2\pi\lambda'$ ,  $a-b$  will be evidently be positive and small, of  $O(\frac{1}{N})$ . Then,  $\psi_{\kappa\mu}$  is small and positive if  $|\kappa-\mu| > 2$ ; small and negative if  $|\kappa-\mu| < 2$  and very large and positive if  $|\kappa-\mu| \approx 2$ .

The last is a consequence of the  $\kappa$  and  $\mu$  differing from integers only by quantities  $O(e^{-N}) \ll \frac{1}{N^2}$  (cf. Sec.IV), such that  $(\frac{\kappa-\mu}{2})^2 - 1 \ll (a-b)^2$  as soon as  $|\kappa-\mu|$  lies in the vicinity of 2. Up to quantities  $O(\frac{1}{N})$ :

$$\psi_{\kappa\mu} = \begin{cases} 0 & \text{for } |\kappa-\mu| > 2 \\ \pi & \text{for } |\kappa-\mu| < 2 \\ \frac{\pi}{2} & \text{for } |\kappa-\mu| = 2 \end{cases} \quad (40)$$

Next, assume  $p-n$  is *odd*. Then for a given  $\kappa$  there are just two values  $\mu = \kappa+1$  and  $\mu = \kappa-1$  for which  $\psi_{\kappa\mu}$  does not vanish, but has the value  $\pi$ . This yields

$$\sum_\kappa \sum_\mu \psi_{\kappa\mu} = 2\pi n. \quad (41)$$

$p-n$  is *even*. For each  $\kappa$  there are 3  $\mu$ 's for which  $\psi_{\kappa\mu} \neq 0$ :

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

Together, this yields once again

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

So,

$$\lambda_1 = \frac{Nk_1}{2\pi} - n = \lambda' - n, \lambda_2 = \lambda_0 + n. \quad (42a)$$

Corresponding for  $Nk_1 = 2\pi(\lambda'+1)$ :

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

$$\lambda_1 = \lambda' + 1 + n, \lambda_2 = \lambda_0 - n. \quad (42b)$$

Thus  $\lambda_1$  ranges over the values,

$$\lambda_1 = n, n+1, \dots, \lambda' - n, \lambda' + n + 1, \dots, N - n. \quad (42c)$$

The  $2n$  values  $\lambda' - n + 1, \dots, \lambda' + n$  are forbidden by the presence of the other spin complexes. Thus, we see that if  $\lambda_0$  is small, then in general  $b > a$ , thus  $\lambda_2 = \lambda_0 - n$ . However,  $\lambda_2$  must be at least equal to  $p$  (see end of preceding paragraph) and therefore,  $\lambda_0 \geq p + n$ . Likewise

<sup>13</sup>We shall see later that for  $a \approx b$ ,  $k_1$  and  $k_2$  in fact have the form  $\frac{2\pi}{N} \times \text{integer}$ , and that therefore  $\lambda_0 = \text{integer}$ .

$\lambda_0 \leq N - p - n$ , from which it follows that if the other spin complex were not present. It is important in both cases that  $n$  be the number of waves of the *smaller* of the two spin complexes. The total number of solutions is, then,

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

The case  $n = p$  remains to be investigated. Here for  $\kappa = n - 1$ , the single partner,  $\mu = \kappa + 2$ , which earlier gave  $\psi_{\kappa\mu} = \frac{\pi}{2}$ , is missing, and for  $\kappa = -(n - 1)$ , the partner  $\mu = \kappa - 2$  is missing, so now

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

In addition, there is now a  $\lambda'$ , so that  $n \cot \frac{\pi\lambda'}{N} = p \cot \frac{\pi\lambda_0}{N}$  and, simply,  $\lambda' = \lambda_0$ . But this does not lead to a solution because whenever  $f_k = f_{\mu}$ ,  $\kappa = \mu$ , and the eigenfunction has already been seen to vanish if two wave numbers are equal. That is,  $k_1$  is at most

$$Nk_1 = 2\pi(\lambda_0 - 1),$$

which yields

$$\lambda_1 = \lambda_0 - \frac{1}{2} - n, \lambda_2 = \lambda_0 - \frac{1}{2} + n;$$

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

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

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

$\lambda_0$  is therefore, obviously, a half integer. Over the range of  $\lambda_1$ , once again  $2n$  numbers are missing:  $\lambda_0 - n + \frac{1}{2}, \dots, \lambda_0 + n - \frac{1}{2}$ , but only  $2n - 1$  in the range of  $\lambda_0$ , so  $\lambda_0$  must equal or exceed  $2n - \frac{1}{2}$  ( $\lambda_2 = n$ ), while it is at most equal to  $N - 2n + \frac{1}{2}$  ( $\lambda_2 = N - 3n + 1$ ), that is,  $\lambda_0$  possesses  $N - 4n + 2$  values instead of the  $N - 2n + 1$  which are allowed when only a single complex of  $n$  waves is present. As interchange of  $\lambda_1$  and  $\lambda_2$  does not affect the solution, the total number of solutions is

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

The situation will perhaps become clearer if, for the moment, we normalized the  $\psi$  differently. Let  $\psi'$  be defined such that, for very large  $a$  it coincides with  $a$ , but for  $a = b$  it remains constant. Then (in the case of two complexes with  $n$  waves,)  $\sum_{\kappa} \sum_{\mu} \psi'_{\kappa\mu}$  grows from zero to  $(2n - 1)2\pi$ , while  $k_1$ , with  $k_2$  fixed, goes from  $\frac{2\pi n}{N}$  to  $\frac{2\pi(N-n)}{N}$ . If

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

then  $\lambda'_1$  clearly takes on all values from  $n$  to  $N - 3n + 1$ , that is  $N - 4n + 2$  values; this also applies to  $\lambda_2$ , with the one restriction, a prohibition against the value which corresponds to  $k_2 = k_1$ .

Now, in general we assume  $q_n$  complexes each with  $n$  waves, that is  $q_1$  single waves with real wave numbers,  $q_2$  pairs with complex conjugate wave numbers, and so on. The constant  $\lambda_1$  of the first of the  $n$  wave complexes could assume any of the values  $n, n + 1, \dots, N - n$ , i.e. take on  $N - 2n + 1$  possible values if there were no other wave-complex present. For each complex with  $p > n$  waves,  $2n$  numbers are lost, as we have seen; for each complex of  $p < n$ , only  $2p$ ; finally, for each of the remaining  $q_n - 1$  complexes with  $n$  waves,  $2n - 1$  numbers. Thus, these are

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

remaining values all allowed for  $\lambda_1$ . The constant  $\lambda_2$  of the second complex of  $n$  waves may not allow  $k_2$  to coincide with  $k_1$ , that is, it has one fewer possibilities; finally, the constant  $\lambda_{q_n}$  of the last complex of  $n$  waves can take on only

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

distinct values, where

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

Finally, considering that interchange of the  $\lambda$ 's of the various wavecomplexes with equal numbers of waves  $n$  does not lead to new solutions, one finds for the total number of solutions

$$\begin{aligned} Z(N, q_1, q_2, \dots) &= \prod_{n=1}^{\infty} \frac{(Q_n + q_n) \cdots (Q_n + 1)}{q_n!} \\ &= \prod_n \binom{Q_n + q_n}{q_n} \end{aligned} \quad (45)$$

where the  $Q_n$  are defined by (44).

## VIII. IMPORTANT IDENTITY

We shall prove now that we have obtained the correct number of solutions. It is known that the number of eigenvalues  $Z(N, r)$  for a fixed value of total spin  $S_{tot} = \frac{N}{2} - r$  equals the number of eigenvalues

with  $M = S_{tot}$  left-handed spins, less the number for  $M = S_{tot} + 1$ , i.e. [1]

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

The following must also hold true

$$\sum_{q_1, q_2, \dots} Z(N, q_1, q_2, \dots) = Z(N, r) \quad (47)$$

the sums being over all values spanned by  $q_1, q_2, \dots$  for which the total number of spin waves equals  $r$ , that is

$$q_1 + 2q_2 + 3q_3 + \dots = \sum_n nq_n = r.$$

In other words, one sums over all the "partitions" of  $r$ ;  $q_n$  gives the number of times the summand  $n$  appears in the particular partition.

We introduce the *total index* of the spin complex

$$q = \sum_n q_n \quad (48)$$

and rewrite (44) as

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

Especially,

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

By E.(45),

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

On the right, next to the binomial coefficient, is the number of allowed solutions with  $q_2$  single spin waves, and generally,  $q_n$  complexes each with  $n-1$  waves in a chain of  $N-2q$  sites. This corresponds to a total of

$$r' = \sum_n q_n(n-1) = r - q \quad (50a)$$

right-handed spins arranged in

$$q' = \sum_{n \geq 2} q_n = q - q_1 \quad (50b)$$

wavecomplexes.

Now we introduce the number of all these solutions, for which  $r$  right-handed spins are arranged in precisely  $q$

wavecomplexes, without distinguishing how many waves each individual complex contains

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

It follows then from (50), (50a), (50b) that

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

and

$$Z(N, r) = \sum_{q=0}^r Z(N, r, q). \quad (53)$$

From here on we treat the problem by complete induction. We assume

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

For  $q=1$  this is certainly correct— we have a single complex of  $r$  waves whose wave numbers can take on  $N-2r+1$  values. Likewise, (54) is correct for  $q=r$ ; then  $q_1=r$  and  $q_n=0$  for  $n>1$  inserted into (45) transforms it into (54). Let us take (54) as proven for  $N-2q, r-q, q-q_1$  and by (52) have

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

Then,

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

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

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

identical with (54). Since (54) holds for  $q = 1$  and for  $q = 2$ ,  $r = 3$  and  $4$ , then for  $q = 2$  and  $r = 3, 4$ , then for  $q = 2$  and greater values of  $r$ , and finally for  $q = 3, 4$ , etc. Inserting (54) in (53) yields

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

in agreement with the number of solutions which we were seeking, Eq.(46). *Therefore, our method yields all the solutions of this problem.*

In a future paper, this method will be extended to space <sup>14</sup> lattices, and its physical implications for cohesion, ferromagnetism and electrical conductivity, will be derived. <sup>15</sup>

## ACKNOWLEDGMENTS

I give my heartfelt thanks to Prof. E. Fermi for especially numerous and stimulating discussions. Also, I thank the Rockefeller Foundation for the grant of a stipend which made my stay in Rome possible.

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<sup>14</sup>three-dimensional

<sup>15</sup>This rash promise has apparently not been kept.