Numerical calculation of two-magnon-states in lower-dimensional Heisenberg ferromagnets
by Robert Peter Reklis

A thesis submitted to the Graduate Faculty in partial fulfillment of the requirements for the degree of
DOCTOR OF PHILOSOPHY in Physics
Montana State University

Abstract:
Numerical techniques are developed to study the two-spin-wave problem in one and two dimensions in finite lattices. Particular emphasis is placed on the bound states formed by the two spin-waves. The results are compared with analytic calculations made for infinite lattices. The assumption that spin-waves are independent and obey Bose statistics is examined and shown to be valid for two spin-waves of small momentum in a class of lattices in one, two, and three dimensions. It is shown that for small total momentum two spin-waves in one dimension may be treated as hard spheres. It is also shown that in two dimensions some of the states which have previously been considered bound can no longer be so considered and that the wave functions as well as the energies of such states must be examined before such a classification can be made. The finite lattice study in two dimensions is accomplished through a manipulation of a diagrammatic notation which is developed here. This technique allows both the energies and wave functions to be calculated. In addition the finite lattice technique allows an examination of the limiting process as lattice size becomes infinite, which is vital to a thorough understanding of the problem.

NUMERICAL CALCULATION OF TWO-MAGNON-STATES IN LOWER-DIMENSIONAL HEISENBERG FERROMAGNETS

by

ROBERT PETER REKLIS

A thesis submitted to the Graduate Faculty in partial fulfillment of the requirements for the degree

of

DOCTOR OF PHILOSOPHY

in

Physics

Approved:

Head, Major Department

Chairman, Examining Committee

Graduate Dean

MONTANA STATE UNIVERSITY
Bozeman, Montana

December, 1973

ACKNOWLEDGMENTS

The author gratefully acknowledges the guidance and encouragement of his advisor, Professor John E. Drumheller. He also wishes to thank Professors John Hermanson, Richard Alben, and Jill Bonner for helpful discussions. Finally, he wishes to thank his wife, Diane Reklis, for her patience and understanding and Peggy Humphrey for her help with typing the manuscript.

TABLE OF CONTENTS

LIST OF FIGURES

ABSTRACT

Numerical techniques are developed to study the two-spin-wave problem in one and two dimensions in finite lattices. Particular emphasis is placed on the bound states formed by the two spin-waves. The results are compared with analytic calculations made for infinite lattices. The assumption that spin-waves are independent and obey Bose statistics is examined and shown to be valid for two spin-waves of small momentum in a class of lattices in one, two, and three dimensions. It is shown that for small total momentum two spin-waves in one dimension may be treated as hard spheres. It is also shown that in two dimensions some of the states which have previously been considered bound can no longer be so considered and that the wave functions as well as the energies of such states must be examined before such a classification can be made. The finite lattice study in two dimensions is accomplished through a manipulation of a diagrammatic notation which is developed here. This technique allows both the energies and wave functions to be calculated. In addition the finite lattice technique allows an examination of the limiting process as lattice size becomes infinite, which is vital to a thorough understanding of the problem.

CHAPTER I

INTRODUCTION TO FERROMAGNETISM

The ability to maintain a magnetic moment by some internal mechanism is a striking feature of ferromagnetic materials. This ability disappears after heating the material past some critical temperature usually denoted T_c. These materials exhibit a crystal structure in which ions are imbedded that have magnetic moments. In a ferromagnetic material there is an energy that cooperatively tends to align these moments. On heating, when the average thermal energy becomes greater than the aligning energy the moments become disordered and the ferromagnetic effect is lost. There are further complications due to domain structures which are not taken into account in the simple model that will be discussed here; the reader need only note that the temperature at which the ferromagnetic property is lost gives an estimate of the aligning energy for one of the ions, $kT_c \tilde{=} J$ the aligning energy.

A considerable mystery developed about the size of this aligning energy that was only cleared up by the advent of quantum mechanics. The aligning forces are too large to be generated by the magnetic fields within the material. This mystery was finally solved by Werner Heisenberg in 1928 [22]. Briefly the argument is as follows. Place two electrons in a potential of the form

the barrier in the center being high enough to form two degenerate states, one centered on the right the other on the left, but low enough to allow some overlap of the wave functions. The wave function for the pair may be written as a spatial part either symmetric or antisymmetric under the interchange of the electrons times a spin part also either symmetric or antisymmetric. The Pauli exclusion principle must be obeyed, so the total wave function must be antisymmetric. Further, the electrons repel each other; thus the states in which the spatial part is antisymmetric have the lower energy, but because of the Pauli principle these states have a symmetric spin part. This difference in energy that the Pauli principle develops between states with symmetric and antisymmetric spin parts may be written formally as a Hamiltonian dealing only with the spin part of the wave function. This spin Hamiltonian,

$$H = -2J\vec{S}_1 \cdot \vec{S}_2$$

is known as the Heisenberg spin Hamiltonian. The J is a constant having units of energy, the $\vec{S}$'s are unitless spin operators and the 2 is added for aesthetic reasons. The exact form of $\vec{S}$ for spin $\frac{1}{2}$ will be given in the next chapter. If J is positive the aligned spin configuration has the lowest energy.

In the above argument only two electrons were used; when doing the full many body problem some complications arise. The sign of J may be

negative. A good discussion of this problem is found in [61]. In any case the Heisenberg Hamiltonian is a suitable starting point in an investigation of ferromagnetism. It is a bit ironic that the forces that align the spins in a ferromagnet are basically electrical and not magnetic in origin. It is also interesting to note that the explanation for ferromagnetism is entirely quantum mechanical. There is no satisfactory classical explanation. There is, of course, the classical mean field argument for ferromagnetic thermodynamics, P. Weiss [52]. This does not explain the aligning energy, however.

The nature of the aligning force has been understood since 1928, the thermodynamics at high temperature away from the critical temperature was explained by Weiss [52] in 1907 and an understanding of the thermodynamics at low temperature away from the critical temperature dates, as shall be seen more fully, from Bloch [3] in 1930. The chief reason that magnetic thermodynamics has been pursued in great depth in the remaining region, temperature near the critical temperature, is the interest in the phase transition.

Phase transitions form a fascinating and mysterious a field of study. Why does water, for example, change from liquid to gas so sharply at one temperature? The gradual change from solid to liquid in glass at least seems to be a more reasonable action on the part of nature.

There seems to be a direct analogy between all types of phase transitions, including the magnetic transition, through the theory of critical exponents. This analogy seems not to be quite exact in the light of recent experiments. However, to a surprising extent the functional forms for thermodynamic quantities are the same for all types of phase transition, differing only with the dimensionality of the substance involved. A reference on the topic of phase transitions [59] is included in the Bibliography. A study of the magnetic phase transition has several advantages. The Heisenberg spin Hamiltonian that is developed above is of simple form and is well understood, unlike the complicated potential between molecules in a gas. Also the magnetic ions are stationary and do not move about as do gas molecules. Further by making alterations to the Heisenberg Hamiltonian a form arises which may be solved exactly in one and two dimensions, namely the Ising model.

The possibility of work in one- or two-dimensional space is also an advantage to the study of the magnetic problem. It is difficult to visualize a one- or two-dimensional real gas, but one- and two-dimensional real magnets are in existence [7, 9, 49, 51]. It is possible to grow crystals in which chains or plates of magnetically interacting ions are widely separated by either water or organic type groups of atoms. The behavior of these materials is very much like that of an ideal one- or two-dimensional magnet. The ability to study phase transitions in lower-

dimensional space yields interesting results: There is no phase transition in one-dimension and in some cases there may not be in two.

The existence of the Ising model solutions [57] in one or two dimensions allows a whole new interaction between physicists. Instead of making comparison only with experiments the theorist who develops a new approximation may test it in the Ising limit in one and two dimensions.

The development of one- and two-dimensional physics is for the most part not an applied topic. A very notable exception lies in the study of two-dimensional domain effects which lies at the heart of the magnetic bubble technology that is now being feverishly studied by the computer industry. Thus lower dimensional studies which might have been considered only a game have considerable scientific and even practical value.

This chapter has presented a very brief overview of the topic of magnetism. No attempt has been made at completeness as there are several adequate texts on the subject, a small list of which is given in the Bibliography. It is hoped that the reader now has a feeling for the relationship between magnetic thermodynamics and phase transitions and an appreciation for lower dimensional physics. In the next chapter an overview of spin-wave thermodynamics will be presented. This is one technique among many used to calculate thermodynamic properties. The

reader who wishes further information on the fascinating topic of magnetic thermodynamics is referred to White [61], Stanley [59], and Huang [57].

CHAPTER II

INTRODUCTION TO SPIN-WAVE THERMODYNAMICS

The basic difficulty in working out thermodynamics in most many-body systems is the large number of states in which the system may be found and which must be dealt with. Magnetism is no exception. Spin-waves were discovered [3] in an attempt to solve the problem of the thermodynamics of magnetism by examining only a few states of the system. The result is valid for low temperatures.

It is convenient at this time to develop a useful identity as follows. The Pauli matrices are usually written

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and find application as a representation of the spin operator for spin $\frac{1}{2}$. This representation of the spin $\frac{1}{2}$ operator must be modified if more than one spin is to be discussed. This is done by introducing a direct product space so that for two spins

$$\sigma_1^x = (\sigma^x \times I) \qquad \sigma_2^x = (I \times \sigma^x),$$

etc. Writing these two matrices out explicitly gives,

$$\sigma_1^x = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \qquad \sigma_2^x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

Then $\vec{\sigma}_1 \cdot \vec{\sigma}_2$ becomes

$$\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y + \sigma_1^z\sigma_2^z$$

which may be written explicitly as

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2 = \begin{pmatrix} 1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1 \end{pmatrix}.$$

The direct product basis states associated with this representation are, $\uparrow\uparrow$ associated with the first row and column through $\uparrow\downarrow$, $\downarrow\uparrow$ to $\downarrow\downarrow$ associated with the last row and column. A permutation of these two spins leaves $\uparrow\uparrow$ and $\downarrow\downarrow$ invariant and takes $\uparrow\downarrow$ into $\downarrow\uparrow$ thus the permutation operator may be written

$$P_{12} = \begin{pmatrix} 1 & & & \\ & 0 & 1 & \\ & 1 & 0 & \\ & & & 1 \end{pmatrix}.$$

Note should be made of the identity

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2 = 2P_{12} - I$$

which is attributed to Dirac and of which extensive use will be made.

The Heisenberg spin Hamiltonian may be thought of as a sum of operators which interchange the spins on neighboring sites. Obviously this does not change the number of up or down spins. Thus the Hamiltonian and the z component of the total spin commute and may be simultaneously diagonalized. Because of this the states may be examined a few at a time. There is only one state that has all the spins spin-up giving the maximum z component. This must be an eigenstate and is the ferromagnetic ground state. There are N states in which there is only one spin spin-down. These states contain the lowest excited states and will be found presently. These are spin-waves. This procedure may be continued in principle until all the eigenstates have been found. So far this has been done only for very small one-dimensional lattices [5].

Because of the difficulty in obtaining eigenstates with many spins down an approximation was made by Bloch [3]. If two spins are turned down in a large lattice Bloch assumed that the spins will in general lie far apart and as only neareste neighbor terms are contained in the Hamiltonian they will not affect one another. This implies that the two-down-spin states may be approximated by the superposition of two one-down-spin states.

In general n-down-spin states may be made up of the superposition of n one-down-spin states so long as n is much smaller than the number of sites in the lattice. Since at low temperatures only the lowest excited states are populated this approximation may be used to determine low temperature thermodynamics.

The one-down-spin states are therefore important. Fortunately they may be easily obtained. It is convenient to generate symmetry in the problem by applying periodic boundary conditions. In one dimension, for simplicity, one may think of a ring of N sites. The boundary conditions of course are unimportant to the low temperature thermodynamics for large N. The Hamiltonian is invariant under a rotation of the labeling of these sites. Further there are N such rotations and they form a group. By analysis of the character table for this group, C_N, one may show that each of the irreducible representations is associated with one state. These representations are one-dimensional and may be written as e^{ik} where $k = 2\pi\lambda/N$ and $\lambda = 1, 2, \ldots, N$. k is, as in band theory, associated with momentum.

That there is a separate k for each state implies that there is a unique representation that diagonalizes these rotation operators. Further since the Hamiltonian is invariant under these rotations the rotation operator and the Hamiltonian may be diagonalized simultaneously; thus one need only find the irreducible representations of the rotation

operators to find the one-down-spins eigenstates. The appropriate eigenbasis is

$$\phi_k = \sum_n \xi(n) e^{ikn}$$

where $\xi(n)$ denotes a down-spin at the n^{th} site. These states are called spin-waves because of their obvious wave-like character, or magnons to stress the particle nature that is dual to the wave nature. This duality will be stressed more fully in Chapter III.

The Two-Spin-Wave State

An obvious question that must be answered at this point is whether Bloch's hypothesis [3] that two down-spins in the lattice behave independently is valid. This question was first addressed by Bethe [2], a year after Bloch put forward his hypothesis in a paper that has proved to be the basis for wide ranging study. Bethe was able to calculate two-down-spin states exactly and was able to generalize to some of the n-down-spin states. His generalization has proved to lead to the ground state for the antiferromagnet (J negative) [24].

The Schrodinger equation for two down-spins may be written as

$$H\psi = E\psi,$$

$$H = -2J \sum_{n,m} \vec{S}_n \cdot \vec{S}_m \quad \text{for n,m labeling neighboring sites}$$

$$= - \sum_{n,m} (P_{n,m} - I/2), \text{ from this in one dimension}$$

$$\xi(m_1,m_2)H\psi = E\xi(m_1m_2)\psi$$

where m_1,m_2 in $\xi(m_1,m_2)$ label the positions of the two down-spins. If $\psi = \sum_{m_1<m_2} A(m_1m_2)\xi(m_1,m_2)$ then the Schrodinger equation becomes

$$A(m_1-1,m_2) + A(m_1+1,m_2) + A(m_1,m_2-1) + A(m_1,m_2+1)$$

$$= EA(m_1,m_2) \quad \text{if } m_2 \neq m_1+1, \text{ or} \tag{1}$$

$$A(m_1-1,m_2) + A(m_1,m_2+1) + 2A(m_1,m_2) = EA(m_1,m_2) \quad \text{if } m_2 = m_1+1 \tag{2}$$

since H is just the sum of nearest neighbor permutations and P_{m_1,m_1+1} interchanges the down-spin at m_1 with the up-spin at m_1+1, etc. It should be noted that a constant factor and many identities have been dropped from the H considered above. The operator P_{ab}, in general, interchanges two up-spins, an identity. There are four exceptions if $m_2 \neq m_1+1$, two if $m_2=m_1+1$. The form for $m_2 \neq m_1+1$ above is just what would be obtained if the two down-spins were independent. The special case $m_2=m_1+1$ is necessary because interchange of the two down-spins at m_1,m_2 is an identity; a nearest neighbor interaction. Bethe [2] proceeded by assigning values to the coefficients A(m,m) so that A(m,m) + A(m+1,m+1) = 2A(m,m+1). Clearly A(m,m) has no correspondence to the physical problem since the

two down-spins may not be at the same site. One of course is free to try to force whatever functional form is chosen for $A(m_1,m_2)$ to have this property. One may or may not be able to obtain a solution to the Schrodinger equation with this property; fortunately for Bethe's technique such solutions exist. If A has this property then Eq. 1 holds even when $m_2 = m_1+1$. Bethe found solutions for A of the form

$$A(m_1m_2) = \exp[i(k_1m_1 + k_2m_2 + \phi/2)] + \exp[i(k_2m_1 + k_1m_2 - \phi/2)] \quad (3)$$

$$\begin{aligned} k_1 &= (2\pi\lambda_1 + \phi)/N \\ k_2 &= (2\pi\lambda_2 - \phi)/N \\ \lambda_1,\lambda_2 &= 1, 2, \ldots, N \end{aligned} \quad (4)$$

$$2 \operatorname{ctn} \phi/2 = \operatorname{ctn} k_1/2 - \operatorname{ctn} k_2/2 \quad (5)$$

This last equation follows from the condition $A(m,m) + A(m+1,m+1) = 2A(m,m+1)$. ϕ may now be eliminated between Eqs. 4 and 5. Not all of the solutions may be obtained in this manner with real k's, however and it is necessary to allow the k's and ϕ to take on complex values to obtain the remainder. These imaginary solutions for the most part have markedly different energies and the down-spins tend to be close together in them. Bethe therefore identified them as bound states. As there is an imaginary solution for all values of total momentum $k_1 + k_2$ Bethe claimed that there was a bound state for all of these values. $k_1 + k_2$ is just the quantum number k for the rotation operator that was discussed earlier.

The appearance of bound states clearly upsets the argument that the down-spins lie far apart and that interactions may be neglected, since the bound states have low energy and will be populated at low temperature. Fortunately the low energy bound states are not tightly bound thus opening the question of their importance to thermodynamics. Many other questions were opened by Bethe's work as well. Are there bound states in two- and three-dimensional lattices? What is the effect of anisotropy and can such bound states be found experimentally? These questions have maintained interest in the bound state problem to the present and are examined in more depth in later chapters.

The question of most obvious importance is the effect on thermodynamics. Spin-wave thermodynamics is dimensionally dependent and it is thus necessary to look separately at one two, and three dimensions. It is easy to derive the relation between energy and momentum k for a spin-wave directly from the Hamiltonian. This relationship is

$$E = A(1 - \cos k)$$

A being a proportionality constant. For small k this becomes

$$E = A(k^2/2 - k^4/24 + \ldots).$$

Keeping only the first term,

$$E = A\, k^2/2.$$

Following Van Kranendonk [60] the zero field magnetization may be derived. The number of spin-waves for any k is given by the Bose distribution,

$$n_k = 1/[\exp(A\ k^2/k_BT)-1].$$

The Bose nature of spin waves is shown in Chapter IV. A knowledge of the deviation from the aligned spin state gives the magnetization,

$$M = M_{aligned} - \text{Deviation}.$$

This deviation is proportional to the total number of spin-waves in the system

$$\text{Deviation} \propto \sum_{\vec{k}} 1/[\exp(A\ k^2/k_BT)-1]$$

In the thermodynamic limit this summation may be taken as an integral so that in three dimensions

$$\text{Deviation} \propto 4\pi \int_{k=0}^{\infty} dk\{k^2/[\exp(A\ k^2/k_BT)-1]\},$$

in two dimensions

$$\propto 2\pi \int_{k=0}^{\infty} dk\{k/[\exp(A\ k^2/k_BT)-1]\},$$

and in one dimension

$$\propto \int_{k=0}^{\infty} dk\{1/[\exp(A\ k^2/k_BT)-1]\}.$$

The resulting integral is convergent only in three dimensions although in two dimensions it is nearly so and the consideration of a slight amount of anisotropy (enhancement of the zz term in the $\vec{S} \cdot \vec{S}$ Hamiltonian) will make it so. Thus, spin-wave thermodynamics predicts that there will be a phase transition in three dimensions and that there will be no transition in one dimension. The result in two dimensions is ambiguous.

Much theoretical work has been done from the high temperature side in two dimensions all of which is ambiguous in the Heisenberg case as to whether a phase transition exists. Mermin and Wagner [31] showed that the magnetic phase does not exist in two dimensions. Stanley and Caplan [45] found that a divergence in the susceptibility could exist, a sure sign of a phase transition. The result of experiment with the best two-dimensional samples [7,9] is to find a magnetic phase but these samples are not perfect two-dimensional magnets. It is clear that a very precise theory is necessary in order to clear up the mysteries in two dimensions. No amount of correction to the spin-wave theory is likely to supply this precision, since if spin-waves are viewed as a gas, thermodynamics may be worked out as a cluster expansion, adding corrections from two-body clusters, three-body clusters, etc., and unfortunately sufficient detail may only be obtained for two spin-waves in the gas (see Dyson [11]).

Thus it appears that in one, two, and three-dimensions spin-waves are a limited thermodynamic tool for a study of the phase transition. Spin-waves have seen application to more complex thermodynamic systems, see [56]. A great deal of interest has been generated in the problems spin-waves present in themselves, which is the business of the next chapters.

CHAPTER III

INTRODUCTION TO TWO-MAGNON INTERACTIONS

The name magnon stresses the particle nature of these excitations and indeed these particles are as real as electrons or protons. If one excites a magnon in a magnetic crystal, he adds a small packet of energy and hence mass, $E = mc^2$. Magnons have momentum and a scattering cross-section can even be calculated [4] for them.[1] In this chapter and the chapters that follow, magnons should be examined on their own; any insight into their thermodynamic origin should be viewed as only an added prize obtained from their study.

There is a great difference between these solid state particles and the more common variety. In studying a magnon there is a preferred frame of reference, that of the lattice. The position of the magnon or its momentum is always relative to the lattice; thus, these are non-relativistic particles. To emphasize the difference examine two electrons in otherwise empty space. There is only one distance parameter that is important; that is the distance between the electrons. It is therefore possible to place the two electrons on a line, one on the right and the other on the left. But rightness and leftness are dependent on how the line is viewed. Interchanging right and left leaves the Hamiltonian

---

[1] See also the discussion of magnon processes in Keffer, Handbuch der Physik, 18, 1 (1966).

invariant and the operator that performs this interchange may be diagonalized simultaneously with the Hamiltonian; further the interchange operator has eigenvalues ± 1. Thus the wave function must have definite parity under interchange. Since the electrons are fermions the parity is antisymmetric. The interaction between the electrons is not easily understood. The interaction between magnons is more easily understood, under certain circumstances they are bosons and this fact may be developed directly from the Hamiltonian as is done in Chapter IV.

Actually it is not always possible to assign a definite parity under interchange of magnons. As may be seen in the above argument this ability in the electron case arose from the relative nature of the problem; only the relative distance between the electrons was important. This is not true in the magnon case. It is certainly possible to reflect the lattice about a point directly between the down-spins and leave the Hamiltonian invariant, but this operation does not commute with the rotation of the lattice. Consequently it is not in general possible to define both the total momentum and the parity under interchange.

A very interesting effect of having two magnons in the lattice is the possibility of forming bound states that was discovered by Bethe [2]. These tend to appear and disappear as total momentum changes; this, of course, is another obvious violation of relativity. These bound states have been thoroughly studied as the problem has from time-

to-time been of interest to many physicists. A short history will be presented here which should provide a guide to the Bibliography of this thesis, as this thesis is largely concerned with bound states. This history will begin with the work of Hanus [21], Wortis [53], and Fukuda and Wortis [19] as their work established the two-magnon problem in its own right. They found the bound state energies of the isotropic Hamiltonian in one, two, and three dimensions. The problem may be pursued along a variety of lines. The complexity of the Hamiltonian may be increased. There is a great interest in anisotropy in magnetism as this is a parameter which yields clearly defined effects in a magnetic material;[2] a classic study of anisotropy is given in Bonner and Fisher [5]. It should be noted that the infinite lattice Heisenberg-Ising problem is near solution in one-dimension [25]. Anisotropy was added to the two-magnon problem in a series of papers beginning with Ovchinnikov [37,38]. Flicker and Leff [15] re-examined Bethe's [2] method and at the same time showed that Bethe's ansatz produced a method which finds all of the states; this was not at all obvious before. Sukiennicke and Zagorski [46] introduced impurities. Silberglitt and Torrance [44], and independently Tonegawa [45] discovered a new variety of bound states introduced by a particular variety of anisotropy.

---

[2]Anisotropy is responsible for hard and easy axes of magnetization and consequently is a strong factor in domain walls.

Another lead is to treat next-nearest-neighbor interactions as this includes the problem of two connected sub-lattices and thus includes the antiferromagnetic problem. A series of papers starting in the fall of 1969 with papers by C. K. Majumdar [30], Lovesey and Balcar [27], and Ovchinnikov [38] studied the problem in one dimension and this work was continued by Oguchi [34, 35, 36] and several others to two dimensions. Majumdar [29] also solved the problem of three magnons in one dimension by applying the technique of Faddeev [13].

Before discussing the experimental work that has been done on the two-magnon problem some of the difficulties of fitting this theoretical work to any experiment should be discussed. The technique that is used in all of the above papers is to impose periodic boundary conditions and partially diagonalize the Hamiltonian with the total momentum quantum number. It may be argued that boundary conditions make no difference to the thermodynamics of a sufficiently large sample. However, boundary conditions may make a great deal of difference to individual wave functions. It is entirely possible that bound states do not exist in the isotropic Heisenberg case with other than periodic boundary conditions.

It is clear that bound states exist in the Ising case.[3] Magnon interactions most certainly exist in either case.

Much experimental work has also been done on the two-magnon problem. Several authors have reported seeing magnon interactions [12,14,30,41]. Torrance and Tinkham [51] were the first to report bound states. They noted multiple g value transitions in $CoCl_2 \cdot 2H_2O$ in the far infared region and were able to explain them quite well with a modified Ising model [50]. The theory was carried forward by Fogedby [16,17,18]. Torrance and Hay [49] have recently reported finding magnon-phonon bound states in $CoBr_2 \cdot 2H_2O$ simultaneously with Ngai et. al. [33] who predicted the magnon-phonon bound state theoretically.

The two-magnon problem has obviously had considerable study both theoretically and experimentally. This author's contribution is presented in the next two chapters. The technique employed is comparatively straightforward and has the advantage that the eigenstates as well as their energies are calculated. The finite lattice technique also allows the manner of approach to the infinite limit to be studied. This is an

---

[3] The Ising Hamiltonian is diagonalized in the direct product representation thus the state represented by "oooxxooo" where the x's represent down-spins is an eigenstate. The pair is well away from the boundary. A linear combination of such states, including states with the pairs on the boundary, must be put together in the Heisenberg case, thus boundary conditions are important.

important advantage as the existence or non-existence of bound states is under certain circumstances difficult to determine. It will be shown that some states that have previously been considered bound are indeed not bound. In the future any theoretical work on the bound state problem will have to consider finite lattice studies. The author believes he has contributed the easiest technique by which this can be done. Also in an attempt to compare the numeric results which were obtained with infinite lattice calculations, light has been shed on the boson nature of the magnons and it is shown that two-magnon bound states are unimportant to thermodynamics in a class of lattices. This helps explain why spin-wave theory is as good as it is in predicting thermodynamic properties for any dimension.

CHAPTER IV

TWO-MAGNON STATES IN ONE DIMENSION[1]

The contribution of the work presented in this chapter is to some extent developmental. The numerical techniques later applied in two dimensions are worked out here. The one-dimensional problem is far easier to solve and there is more previous work available for comparison. Bethe's work is constantly referred to. Particular emphasis is placed on the bound states which are the easiest to study. The work presented here also includes some previously unknown results. The assumption that spin-waves are to a large degree independent and obey Bose statistics at low temperatures is proved for a class of lattices in one, two, and three dimensions. This implies that the two-magnon results will not be important to thermodynamics for lattices in this class, as was shown by Dyson in three dimensions. It is shown in the one-dimensional problem that for small total momentum two spin-waves may be treated as hard spheres. An interesting oscillatory effect is also observed in the wave functions for the bound states. This seems to be characteristic of the periodic boundary conditions and reappears in Chapter V dealing with two-dimensional lattices.

---

[1] Material in this chapter is largely taken from [40].

Analysis of the Hamiltonian

The spin Hamiltonian for the Heisenberg ferromagnet arranged in a ring of N spins is

$$H = -2J\,\vec{S}_1 \cdot \vec{S}_N - 2J \sum_{m=1}^{N} \vec{S}_m \cdot \vec{S}_{m+1} ,$$

where the exchange energy is J, and the spin operator for the i^{th} site is $\vec{S}_i$.

By using the Dirac identity the Hamiltonian for spin $\frac{1}{2}$ may be written as

$$H = J[\tfrac{1}{2}NI - (N-4)I - H_1],$$

$$H_1 = -(N-4)I + P_{1,n} + \sum_{m=1}^{N-1} P_{m,m+1},$$

where I is the identity operator and $P_{i,j}$ interchanges sites i and j.

Rotating the labeling of the sites (m goes to m+1) leaves the Hamiltonian invariant and this operator R commutes with the operator for the z component of the total spin. It is convenient to represent the Hamiltonian in a basis which diagonalizes both the operator R and the z component of the total spin. Satisfying these requirements for the states with all spins up except for one turned down produces eigenstates of the Hamiltonian.[2] For states with two overturned spins in a ring

---

[2] As in Chapter II.

with N odd,[3] a set of basis states which meets these requirements but does not diagonalize H is

$$\phi_r = [\sum_{m=1}^{N} \xi(m,m+r)\exp(ikm)]/N^{\frac{1}{2}},$$

where

$$r = 1, 2, \ldots, (N-1)/2;$$

$$\xi(m_1,m_2) = (\alpha_1\alpha_2 \cdots \alpha_{m_1-1}\beta_{m_1}\alpha_{m_1+1} \cdots \alpha_{m_2-1}\beta_{m_2}\alpha_{m_2+1} \cdots \alpha_N);$$

$$k = 2\pi\lambda/N;$$

$$\lambda = 1, 2, \ldots, N.$$

In this basis H_1 becomes block diagonalized with N blocks of the form

$$H_1 = \begin{bmatrix} 2 & 1+\exp(-ik) & & & & \\ 1+\exp(ik) & 0 & 1+\exp(-ik) & & & \\ & 1+\exp(ik) & \cdot & \cdot & & \\ & & \cdot & \cdot & 1+\exp(-ik) & \\ & & & 1+\exp(ik) & 0 & 1+\exp(-ik) \\ & & & & 1+\exp(ik) & F \end{bmatrix}_4 \quad (1)$$

where H_1 contains (N-1)/2 rows and columns and $F = (-1)^{\lambda}2\cos(\frac{1}{2}k)$. It should be noted that there are N values for k and (N-1)/2 states for each value. This gives the correct number of states.

---

[3] See Appendix II for an example of the difference between odd and even lattices.

[4] This form is calculated for N=5 explicitly in Appendix II.

The permutation operators in H_1 may increase or decrease r by one. For this reason only immediately off-diagonal elements of H_1 are non-zero. The matrix H_1 treats all basis states equally except for the first and the last. The first is a special case because both overturned spins are neighbors and only two of the permutation operators in H_1 take this state out of itself. Similarly for the states in which the overturned spins are as far apart as possible, only two of the permutation operators in H_1 give states in which the two overturned spins are not as far apart as possible.

A few comments will suffice here for the case of the ring with even N.[5] Two H_1 matrices are developed. If $\exp(-ikN/2) = -1$, a matrix similar to Eq. 1 is obtained with (N/2)-1 rows and columns, and F = 0; while if $\exp(-ikN/2) = +1$, there are N/2 rows and columns, F = 0, but the lowest non-diagonal components are adjusted by a factor of $\sqrt{2}$.

For one particular value of k ($k=\pi$) the matrix form of H_1 is diagonal with an eigenvalue of 2 corresponding to the state in which the two down-spins are neighbors and all the other eigenvalues are 0. For $k=\pi$ there is clearly a bound state of binding energy 2. Figure 1 gives the eigenvalues of H_1 as a function of k for a ring of 31 spins. These eigenvalues were found by developing the characteristic polynomial from a recursion relation and solving it numerically. The details of this calculation are given in Appendix I and are similar to the procedure used by Torrance and Tinkham [50].

[5] See also Appendix II for N=4.

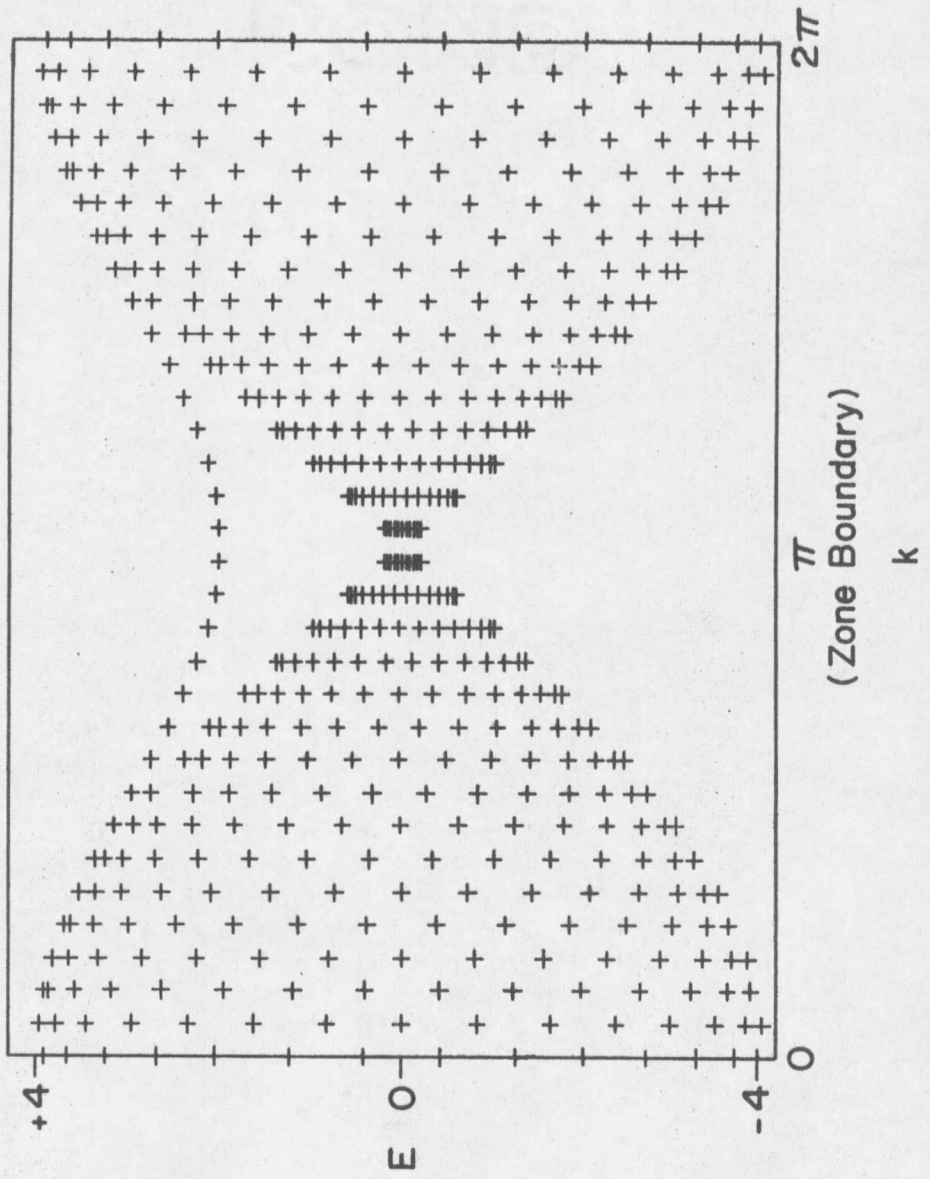


Fig. 1. Eigenvalues of H_1 as a function of total momentum (k) for a ring of 31 spins.[1]

Bound States

The bound states are clearly defined for k near π, as may be seen in Figure 1. For k near 0 they are not so well defined and further analysis is necessary in this region. A feature of the bound states that may be exploited near k=0 is their radii, $\bar{r}(k)$, the average distance between the two down-spins. This may be written as

$$\bar{r}(k) = \sum r_i P_i(k) ,$$

where r_i is the distance between the two down-spins and $P_i(k)$ is the probability that the down spins are r_i apart. The $P_i(k)$ can be calculated from the standard probability interpretation of the eigenvectors. As the bound states correspond to the largest eigenvalues of H_1, the eigenvectors can readily be calculated [55].

In Figure 2 the radii of the states corresponding to the largest eigenvalues are shown as a function of k for a ring of 101 spins. There are two obvious envelopes for k near 0. The end points of these envelopes at k=0 are calculable. The upper end point is N/4. This corresponds to a perfectly random placement of the two down-spins. If all possible radii are equally probable the average will be N/4, as the two down-spins can be no farther apart than N/2. In Figure 3 the end of the lower envelope is examined. It assumes a value slightly less than 0.15 for $N=\infty$.

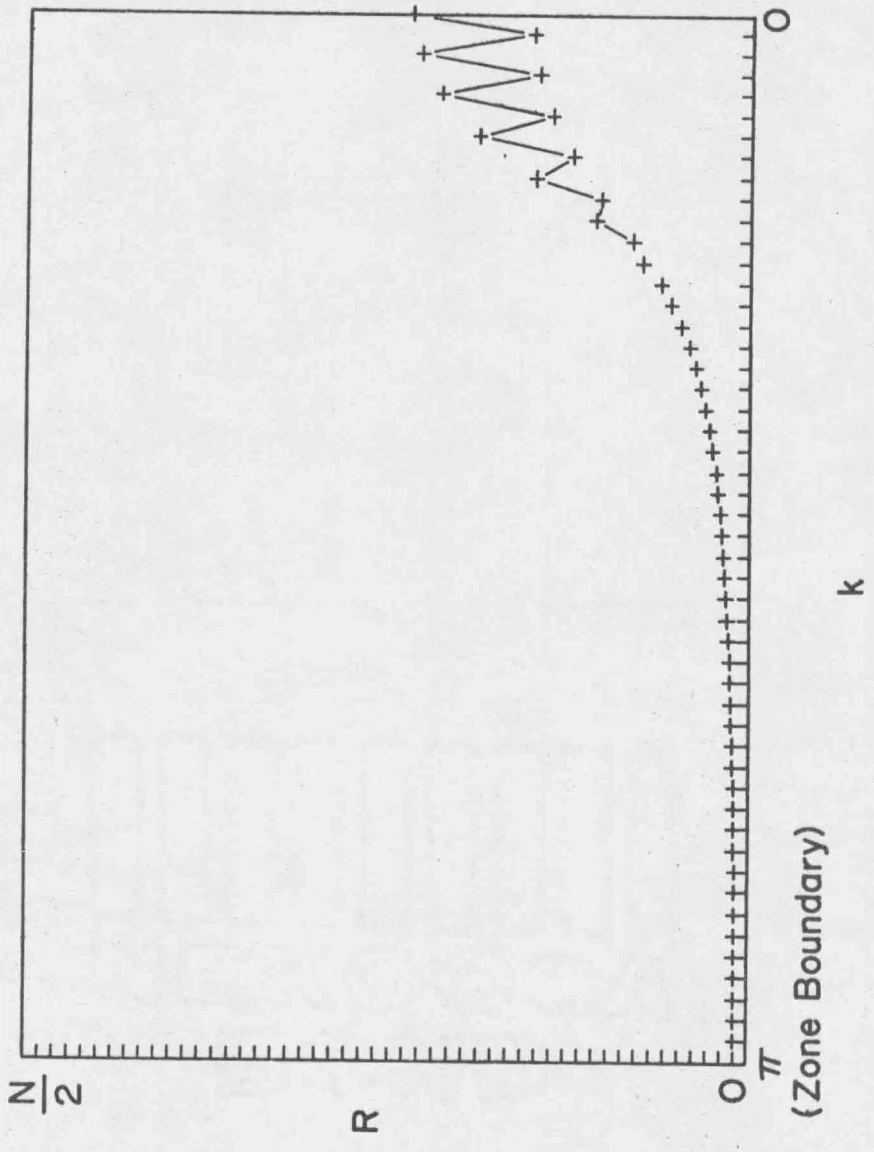


Fig. 2. Radii of states of H_1 with highest eigenvalue (these include any possible bound states) as a function of total momentum (k) for a ring of 101 spins.

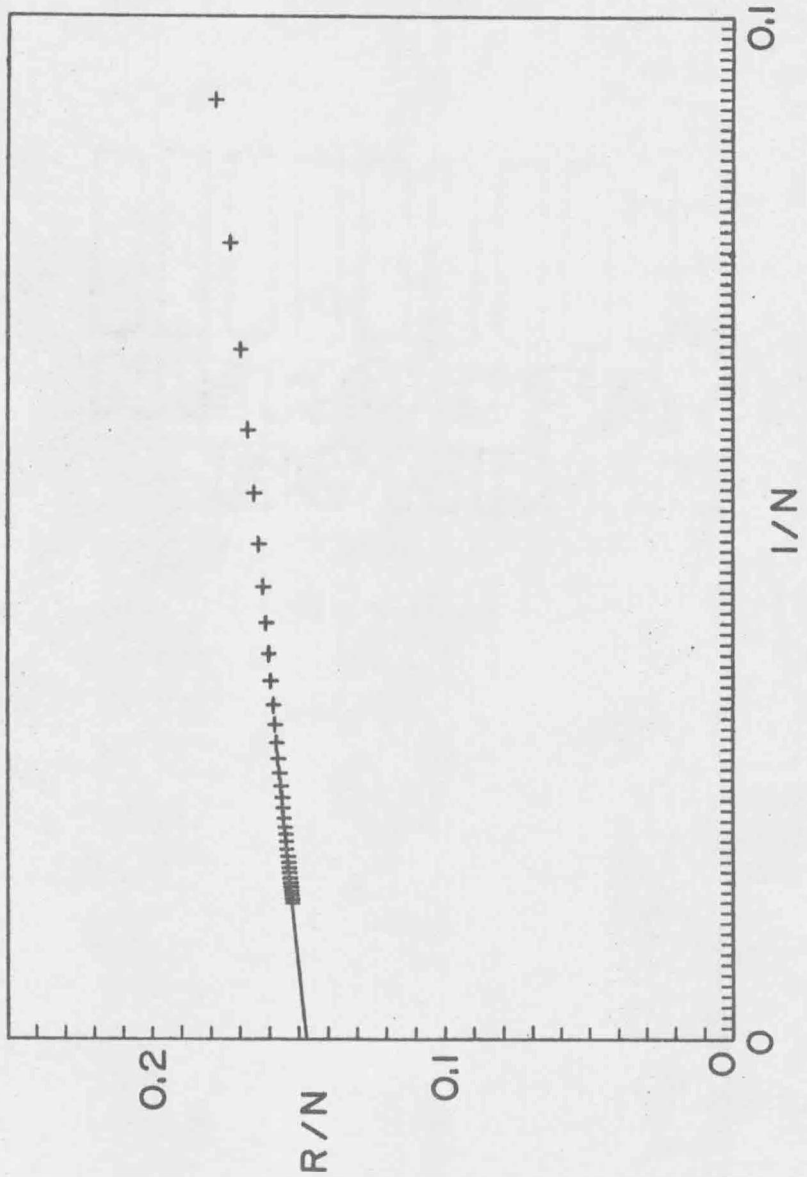


Fig. 3. Radii of states of H_1 with highest eigenvalue when $k=2\pi/N$ as a function of 1/N for rings with N spins. This shows the end of the lower envelope in Fig. 2 and allows interpolation as N becomes large.

Analytic Calculation at Small k

An approximation which follows Bethe's technique can be developed from which this value may be calculated. Assuming a solution of the form

$$\psi = \sum_{m_1>m_2} A(m_1,m_2)\ \xi(m_1,m_2)\ .$$

The coefficients A may be determined by writing the eigenvalue problem for H_1 as

$$A(m_1-1,m_2) + A(m_1+1,m_2) + A(m_1,m_2-1) + A(m_1,m_2+1) = E\ A(m_1,m_2), \quad (2)$$

with the condition

$$2A(m,m+1) = A(m,m) + A(m+1,m+1).^{6} \quad (3)$$

This condition allows Eq. 2 to be used when the down-spins are nearest neighbors. By subtracting 2A(m,m) from Eq. 3 a difference equation is obtained. Then if A does not change significantly from one lattice site to another, by using the standard definition of a derivative, the above condition may be written in derivative form as

$$2\frac{d}{dx} A(m,x)\Big|_{x=m} = \frac{d}{dx} A(x,x)\Big|_{x=m}\ .$$

Again using standard definitions, this becomes

---

[6] This argument is carried out in further detail in Chapter II.

$$\frac{d}{dx} A(m,x)\Big|_{x=m} = \frac{d}{dx} A(x,m)\Big|_{x=m}. \qquad (4)$$

As the form of Eq. 4 is symmetric with respect to x and m it is satisfied if $A(m_1,m_2) = A(m_2,m_1)$.

Making this assumption, the solution for the energies becomes

$$E = 2\cos(k_1) + 2\cos(k_2) ,$$

and for the coefficients becomes

$$A(m_1,m_2) = \exp[i(k_1m_1+k_2m_2)] + \exp[i(k_2m_1+k_1m_2)]$$

$$= 2\exp[i(k_1+k_2)(m_1+m_2)/2] \cos[(k_1-k_2)(m_2-m_1)/2] ,$$

with

$$k_1 = 2\pi\lambda_1/N,\ k_2 = 2\pi\lambda_2/N,\ \lambda_1,\lambda_2 = 1, 2, \ldots, N .$$

The coefficients A correspond to symmetric plane waves and therefore the solution is that of a noninteracting Bose gas. The calculation of the radius then becomes

$$R = \int_0^{N/2} dr\ r \cos^2[(k_1-k_2)r/2] \Big/ \int_0^{N/2} dr \cos^2[(k_1-k_2)r/2] .$$

This yields

$$R = \begin{cases} N/4, \ \lambda_1-\lambda_2 \text{ even, end of upper envelope,} \\ N(1/4-1/\pi^2), \lambda_1-\lambda_2 = 1, \text{ end of lower envelope.} \end{cases}$$

The value $N(1/4-1/\pi^2) = 0.1487N$ compares favorably with the result of the numerical calculation, $<0.15N$. Bethe [2] developed expressions for the eigenvalues and eigenvectors of the bound states and a naive calculation based upon those results leads to a value of N/8 for the end of the lower envelope. The difference between the above calculation and Bethe's work is in the point at which the approximation is made. This was done as Bethe's technique for examining the bound states is not easily applied to very small k. It should be emphasized that the solution for small k_1 and k_2 presented above is an exact solution to the problem as set up by Bethe and as may be seen from the agreement with the numerical calculation, any possible bound states are included.

Other Lattices

Expressions similar to Eqs. 2 and 3 may be readily obtained for any lattice in which the exchange interaction is J between nearest neighbors, is zero otherwise, and all lattice sites are equivalent. The differential condition of Eq. 4 becomes a set of equations with derivatives taken along all vectors that connect nearest neighbors. These conditions can be satisfied by insisting that the solution has the Bose property, and the equation corresponding to Eq. 2 can be solved by assuming that the two down-spins behave independently. Consequently bound states, and indeed any interaction between the spin-waves, may be ignored if the two moments $\vec{k}_1$ and $\vec{k}_2$ corresponding to the two spin-waves are small. This is the region

in which lack of interaction between the spin-waves is important to thermodynamic calculations at low temperature.

There are three points in relation to the above argument that must be discussed. First, it must be established that equations of the form 2 and 3 have solutions for other than the one dimensional lattice. Second, if there are solutions there is no guarantee that all of the solutions to the two-spin wave problem may be found in this manner even at small $\vec{k}_1, \vec{k}_2$. Third, spurious solutions may be generated by the approximation leading to Eq. 4.

The first point poses no difficulty in one small $\vec{k}_1, \vec{k}_2$ limit as the noninteracting Bose gas is a solution in this limit. The second point creates more difficulty. The noninteracting Bose gas approximation gives too many solutions in all; from this it may be argued that the approximation overlooks at most a few states at small $\vec{k}_1, \vec{k}_2$. This would leave the thermodynamic calculations undisturbed. In the one dimensional lattice no states are overlooked. As to the third point the approximation leading to Eq. 4 becomes exact for small $\vec{k}_1, \vec{k}_2$.

Wortis [3] calculated the energy of the bound states in the two-dimensional square lattice and in the three-dimensional cubic lattice. He found that the bound states vanish at $\vec{k}_1 = \vec{k}_2 = 0$. This is certainly in agreement with the above result.

Hard Spheres

In one dimension there are $N^2/2$ different pairs k_1,k_2 whereas there are $N(N-1)/2$ different states. An easy way to eliminate the excess states is to choose the total momentum $k=k_1+k_2$ in N ways and k_2 in N-1 ways.

$$k=2\pi\lambda/N,\ \lambda = 1, 2, \ldots, N,$$

$$k_2=2\pi\lambda_2/(N-1),\ \lambda_2 = 1, 2, \ldots, (N-1),$$

$$E=2\cos(k-k_2)+2\cos(k_2). \tag{5}$$

The essence of this approximation is that the degree of freedom for the second spin-wave inserted in the lattice is one less than the degree of freedom of the pair. That is, the spin-waves behave as hard spheres. This scheme introduces a spurious double degeneracy for each energy which is easy to accommodate by dividing by two. Figure 4 shows Eq. 5 plotted with k as a continuous variable for all values of k_2. These curves are superimposed on the exact solution. The value of N in Figure 4 is 31. Quite good agreement between the hard sphere approximation and the exact solution for a large range of k results.

Bethe [1] approached the two spin-wave problem by assuming a solution to Eqs. 2 and 3 of the form that gives for the coefficients

$$A(m_1,m_2) = \exp[i(k_1m_1+k_2m_2+\phi/2] + \exp[i(k_2m_1+k_1m_2-\phi/2)] \tag{6}$$

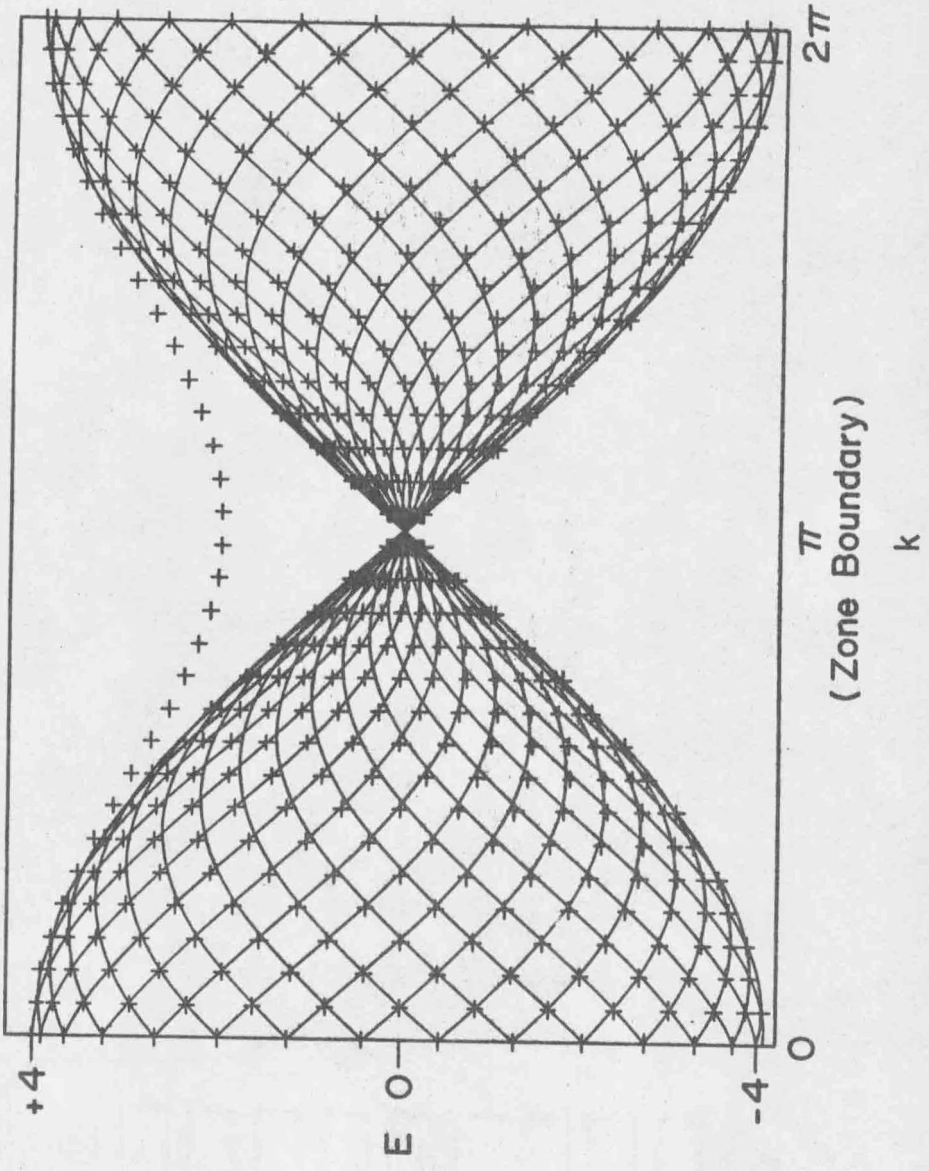


Fig. 4. A comparison of the hard sphere approximation with the exact solution for 31 spins shown in Fig. 1. If the hard sphere approximation had been exact the continuous lines would pass through the crosses.

and for the energies

$$E = 2\cos(k_1) + 2\cos(k_2),$$

with

$$k_1 = (2\pi\lambda_1 + \phi)/N,$$

$$k_2 = (2\pi\lambda_2 - \phi)/N.$$

The condition Eq. 3 then becomes

$$2\mathrm{ctn}(\phi/2) = \mathrm{ctn}(k_1/2) - \mathrm{ctn}(k_2/2).$$

For k=0 this becomes

$$\phi = -2\pi\lambda_2/(N-1)$$

and

$$k_2 = 2\pi\lambda_2/(N-1).$$

Thus the hard sphere approximation gives exact energies for k=0. The spin-waves are bosons only for k_2 small as can be seen from Eq. 4. Only with k_2 small can m_1 and m_2 be interchanged in Eq. 6. In this limit the hard sphere approximation is equivalent to the noninteracting approximation so that there is no contradiction with it.

CHAPTER V

NUMERICAL CALCULATION OF TWO SPIN-WAVE BOUND STATES IN SOME TWO-DIMENSIONAL HEISENBERG FERROMAGNETS[1]

In this chapter the techniques developed in the last chapter to study the bound states are carried over into two dimensions. The contribution made by the work in this chapter is also developmental in part and also produces results of immediate interest. The difficulty in making the transition from one to two dimensions lies largely in obtaining a suitable basis. A notation is developed in this chapter to obtain and manipulate basis vectors for two-dimensional or higher dimensional lattices although work in three dimensions is probably impractical. It should be possible to extend this scheme to other problems in two dimensions, however. The result of most immediate interest achieved by this work is to show that states that have been considered bound up until this time can no longer be so considered. This result should be of interest to others working on the two-magnon problem because it demonstrates that the wave functions as well as the energies are important in determining whether states are bound or unbound and that the manner of approach to the thermodynamic limit is also of interest. The author feels that he has contributed a clear and elegant method for pursuing a knowledge of the bound state wave functions and the manner in which the bound state solutions approach the thermodynamic limit.

---

[1] Material in this chapter is largely taken from [39].

The Hamiltonian

As before the Heisenberg spin Hamiltonian for a ferromagnet is given by

$$H = -2J \sum_{\langle m,n \rangle} \vec{S}_m \cdot \vec{S}_n ,$$

where the exchange energy is J and the operator for the spin on the n^{th} site is $\vec{S}_n$. The sum is taken over all nearest neighbor pairs m,n in the crystal lattice. The Hamiltonian may be written in terms of permutation operators for the spin $\frac{1}{2}$ case using the Dirac identity

$$\vec{\sigma}_m \cdot \vec{\sigma}_n = 2P_{m,n} - I,$$

in which $P_{m,n}$ is an operator that permutes sites m,n. It is convenient to introduce a dimensionless Hamiltonian

$$H_1 = \sum_{\langle m,n \rangle} P_{m,n} - (N/2-2)Iz,$$

so that

$$H = -JH_1 - J(N/2-2)Iz + JIzN/4,$$

where z is the coordination number of the lattice (the number of nearest neighbors for any lattice site) and N is the number of lattice sites.

Application of Periodic Boundary Conditions

In the one-dimensional problem with periodic boundary conditions imposed, the operator which rotates the labeling of the lattice sites (m goes to m+1, N-1 goes to 0) is a diagonal in the basis

$$\phi_r = [\sum_{m=0}^{N-1} (m,m+r)\exp(ikm)]/N^{\frac{1}{2}}, \qquad (1)$$

where

N is odd;

$r = 1, 2, \ldots, (N-1)/2$;

$\xi(m_1,m_2) = (\alpha_0, \alpha_1, \ldots, \alpha_{m_1-1}, \beta_{m_1}, \alpha_{m_1+1}, \ldots, \alpha_{m_2-1}, \beta_{m_2}, \alpha_{m_2+1}, \ldots, \alpha_{N-1})$;

$k = 2\pi\lambda/N$;

$\lambda = 1, 2, \ldots, N$.

$\xi(m_1,m_2)$ defines the position of the two down-spins. In this basis k is a good quantum number, e^{ik} is the rotation operator, and the Hamiltonian mixes only states with the same k.

The basis states, Eq. 1, are defined by the value of k and the distance between the two down-spins. It is necessary to generalize this type of basis to two-dimensions which may be done by introducing a diagramatic notation. The diagram

x o x o o

describes the state in which the two down-spins, marked with an x, are separated by one up-spin for a ring of five sites, the value of k being arbitrary. It is possible to choose these diagrams in such a way that one down-spin is always on the first site. It is clear that there is an equivalence between

x o x o o and x o o x o

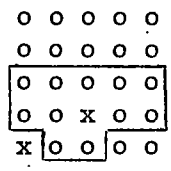
since in either case the two down-spins are separated by one up-spin. In the diagrams the first and last sites are adjacent due to the periodic boundary conditions. Because of the possibility of equivalent diagrams care must be taken in making up a basis so that only non-equivalent diagrams are used. A basis for the ring of five sites is

x x o o o

x o x o o.

Every possible value of k must be associated with each of these diagrams.

Generalizing to two dimensions for a 5x5 square lattice the basis states may be represented by diagrams of the form



Once again care must be taken to include only non-equivalent diagrams in a basis set. The area enclosed by the line on the above contains all possible non-equivalent positions for the second down-spin, the first always being placed in the lower left-hand corner. A further discussion of these diagrams is given in Appendix IV. This is not a unique scheme for obtaining all non-equivalent sites for the second down-spin. It should be noted, nevertheless, that this scheme gives $(n^2-1)/2$ non-equivalent diagrams for an nxn square lattice. Each set of such diagrams is associated with a k_x and k_y which are quantum numbers for rotations in the x and y directions respectively. There are n^2 different values for k_x and k_y; this gives a total of $n^2(n^2-1)/2 = N(N-1)/2$ where N is the total number of sites. This is exactly the dimension of the vector space associated with the Hamiltonian. The diagrams then represent a set of linearly independent states the number of which is the same as the dimension of the Hamiltonian and consequently the diagrams represent a basis.

The Hamiltonian in the form H_1 contains the sum of the permutations of all nearest neighbor sites. The effect of H_1 on a state represented

by one of these diagrams is to move the locations of the two down-spins to any neighboring sites. The rotation operators must be applied to regain a diagram of the form contained in the basis set when the corner spin is moved. As an example, in one dimension H_1 applied to the diagram

x o x o o o o

gives

$$(1+e^{-ik})\ x\ x\ o\ o\ o\ o\ o + (1+e^{ik})\ x\ o\ o\ x\ o\ o\ o.$$

Note that all of the permutations which give the identity when applied to these diagrams have been subtracted out in forming H_1.

When the down-spins are neighbors, the two permuations that would otherwise move them closer together only interchange them leaving the state unchanged. For this reason the diagrams in which the spins are neighbors must be dealt with as a special case. Another special case arises when the Hamiltonian is applied to diagrams in which the second down-spin is at a site on the border containing the non-equivalent diagrams. The Hamiltonian may be applied to these states by associating the diagrams for the second spin immediately outside the boundary with the appropriate ones for the second spins inside, to which they are equivalent.

Obtaining the Bound States

Bound states for each pair of k_x, k_y if they exist will have the highest eigenvalues of H_1. This enables a simple technique to be used

in finding them [55]. If a particular state is a linear combination of two eigenstates then

$$H^n(a_1|E_1\rangle + a_2|E_2\rangle) = E_1^n\, a_1|E_1\rangle + E_2^n\, a_2|E_2\rangle .$$

If $E_1 > E_2$ the right-hand side is

$$E_1^n\, [a_1|E_1\rangle + (E_2/E_1)^n a_2|E_2\rangle],$$

and in the limit $n\to\infty$ this becomes

$$E_1^n\, a_1|E_1\rangle.$$

Thus the application of the Hamiltonian a sufficient number of times effectively projects out the state with the highest eigenvalue. It is easiest of course to carry out this procedure with a computer.

A matrix representation for the block of the Hamiltonian, for any k_x, k_y, would be of dimension (N-1)/2, where N is the total number of sites. For a 25x25 square lattice this is 312. A matrix of this dimension contains 10^5 entries which is too large to manipulate even with a computer. Fortunately the calculation can be performed without writing the Hamiltonian as a matrix since the operation of the Hamiltonian on the basis diagrams shown above is of a simple form.[2]

---

[2] Details of the computer programming are given in Appendix V.

Results

Table I gives a comparison between the results of Wortis' formula for the two-dimensional square lattice, suitably modified, and the energy obtained numerically herein for a 25x25 lattice. As the energy lies above the continuum along $k=k_x=k_y$ for every k except k=0 Wortis also held that a bound state existed for every k except 0. The numerical technique developed in the previous sections also determines the eigenvector which can be interpreted in the usual way to obtain the probability that the two spins will be separated by Δx and Δy, and from this the average separation may be obtained. The average Δx ($\overline{\Delta x}$) is plotted in Figure 5 as a function of $k=k_x=k_y$ for n=25. It should be noted that the average separation oscillates as k approaches 0 and that for some values $\overline{\Delta x} = n/4 = 6.25$. If the arrangement of the two down-spins was completely random $\overline{\Delta x}$ would be n/4. This is because the periodic boundary conditions restrict the two down-spins to be separated in the x direction by no more than n/2. A random $\overline{\Delta x}$ would give the average as n/4. As the average separation is greater than the random separation the interaction between the magnons for some values of k must be considered repulsive. The origin of the repulsive interaction is discussed in Section VII.

It is a good approximation to assume that the magnons are independent Bose particles when their individual moments are small, and also that bound state behavior is unimportant for small total momentum vectors. Figure 6 shows the surface on which the highest eigenvalues

Table I. Highest Eigenvalues of States with $k_x=k_y=k$ for the Periodic Square Lattice.

k	Wortis formula infinite lattice	Numerical 25x25	Difference
0	8.0000	8.0000	0.
$2\pi/25$	7.9369	7.9298	0.0071
$4\pi/25$	7.7487	7.7491	-0.0004
$6\pi/25$	7.4382	7.4315	0.0067
$8\pi/25$	7.0104	7.0124	-0.0020

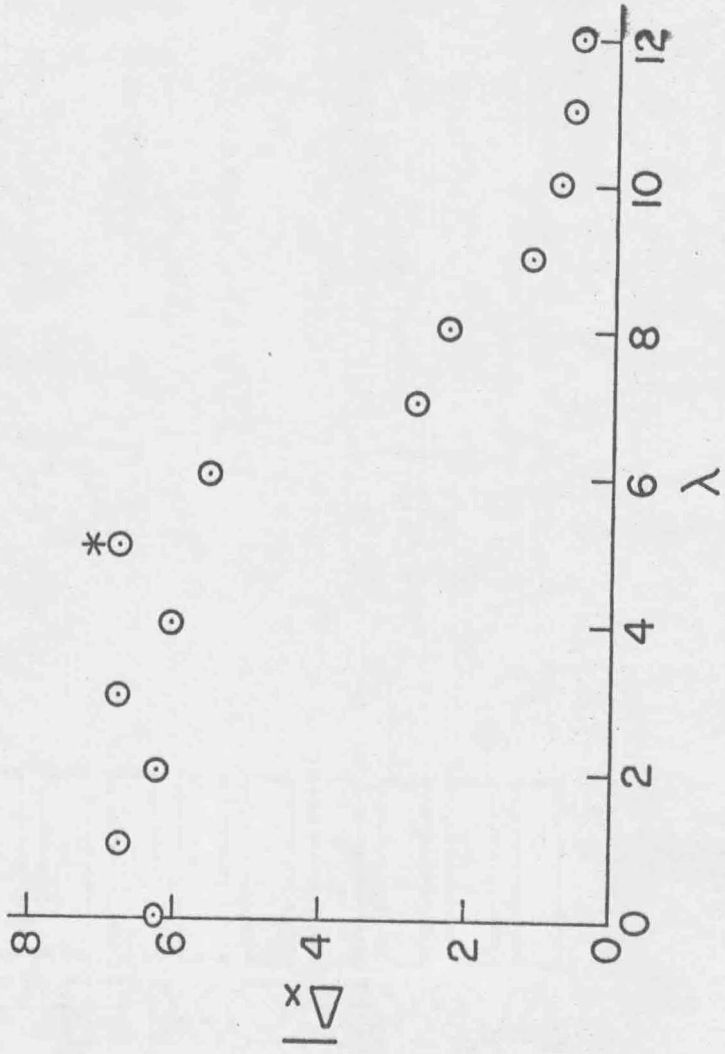


Fig. 5. Average separation of down-spins in the x direction as a function of $k=k_x=k_y$ for a 25x25 square lattice. On these plots $k=2\pi\lambda/n$ the lattice being nxn. The point marked with the asterisk did not meet the convergence criterion.

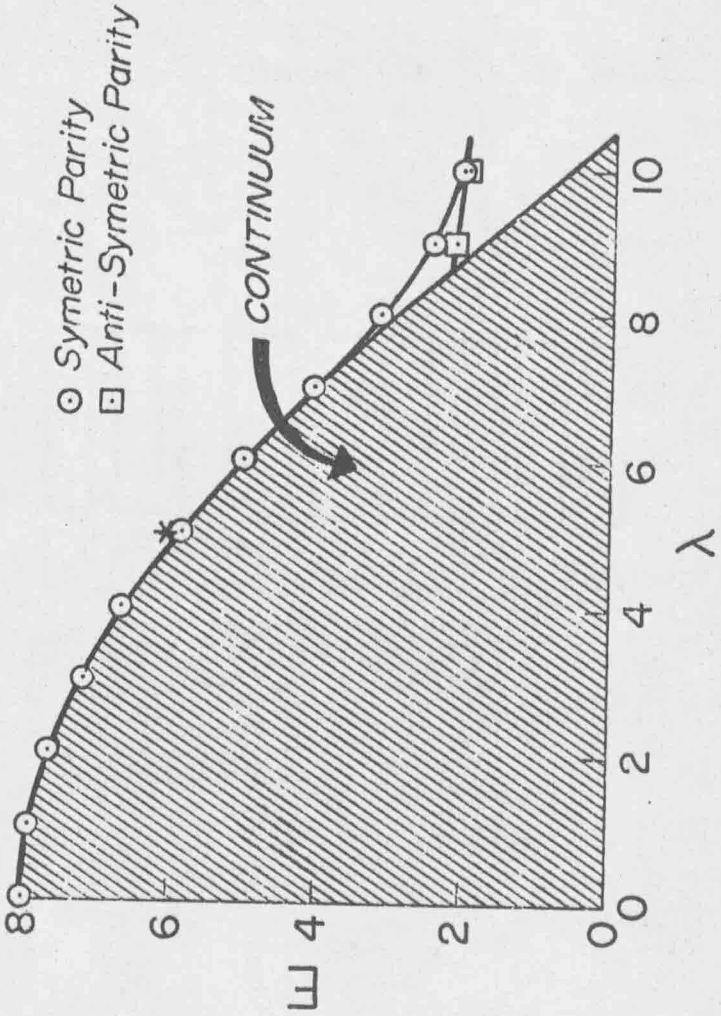


Fig. 6. The highest eigenvalue as a function of total momentum in the x and y directions. Note that the second lower bound state is omitted in this figure.

of H_1 lie and Figure 7 shows the bound state energies along $k=k_x=k_y$. As may be seen in these two figures the bound states for small $\vec{k}$ are close to the continuum if they exist at all.

Wortis was able to show that in some portions of the Brillouin zone there were two bound states. It is easy to show that at the corner of the zone the two states in which the two down spins are nearest neighbors are eigenstates with eigenvalue 2. Further, one may insist that all states in which $k_x=k_y$ must have either even or odd parity when the x and y axes are interchanged. At the zone corner the even and odd states may be constructed from the two states in which the down-spins are neighbors and are degenerate. It is possible to include only states with even or odd parity when applying the numerical techniques described above and to obtain both bound states when $k_x=k_y$. The eigenvalues for both even and odd parity are shown in Figure 7.

Triangular Lattice

By connecting sites in a parallelogram with acute corners of 60° by a triangular lattice a structure is formed to which periodic boundary conditions may be applied. Quantum numbers k_x and k_y may be formed for this lattice so that e^{ikx} and e^{iky} are operators that shift the lattice one row in the x or y directions as shown in Figure 8. At no point in k space does the spin-wave continuum condense to a single energy as is the case for the square lattice and the one-dimensional lattice. It is

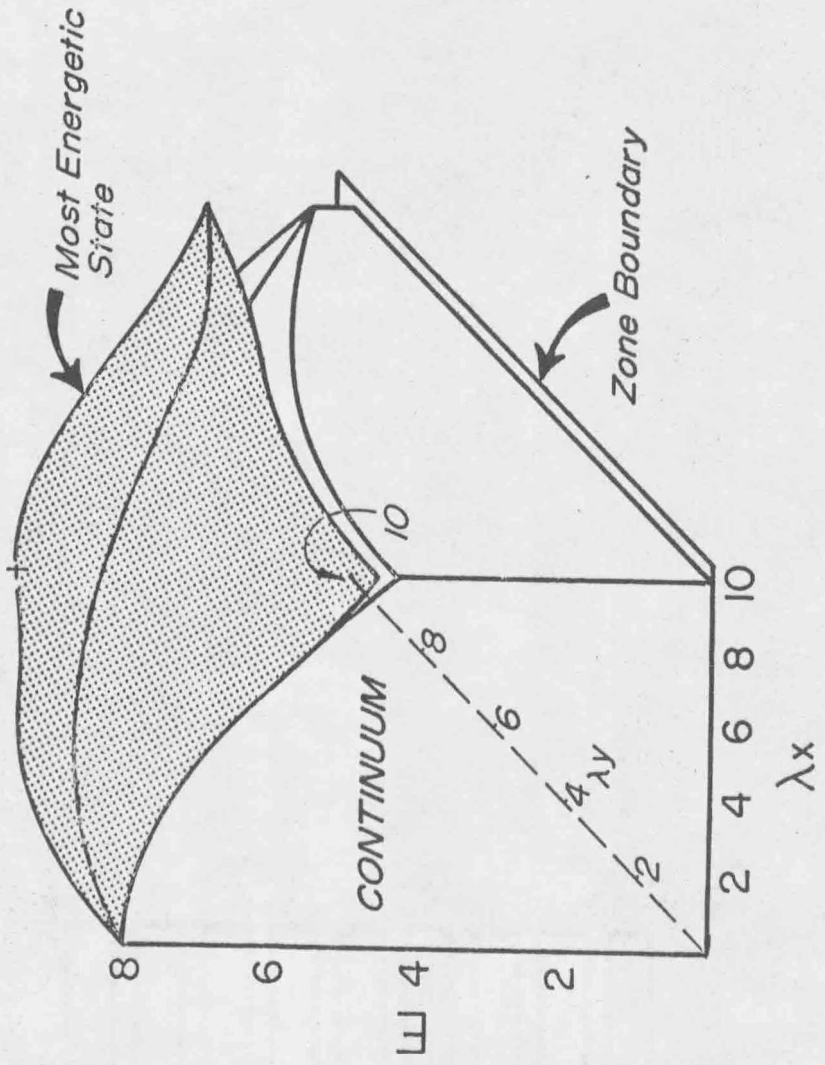


Fig. 7. Bound state energies as a function of $k=k_x=k_y$, $k=2\pi\lambda/n$. The points plotted are for n=21. Parity refers to the transformation properties of the state as the x and y axes are interchanged.

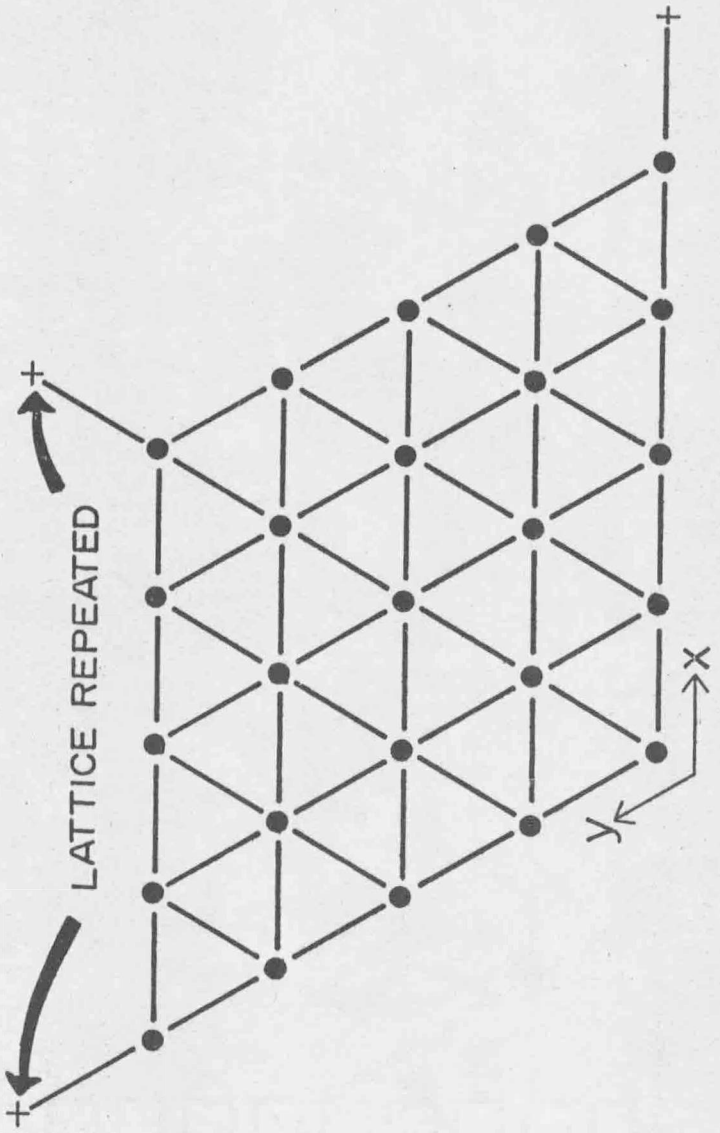


Fig. 8. This diagram shows the way in which periodic boundary conditions were applied to the triangular lattice.

at this point of condensation that the magnons are most nearly bound. Consequently, the existence of bound states in the triangular lattice may be questioned. Figure 9 shows the highest energy state along a line in k space $k=k_x=k_y$ and Figure 10 shows the corresponding radius. Throughout the region in which the difference between the continuum and the bound state is greatest a study of the radius shows that the magnons repel each other. There is a real bound state at the corner, however.

The Repulsive Force

The origin of the repulsion between the two magnons may be seen most easily in one-dimension. The Hamiltonian H_1 is block diagonalized in the basis of Eq. 1 and the blocks for each k may be written as [5]

$$\underline{\underline{H}}_1 = \begin{bmatrix} 2 & 1+\exp(-ik) & & & & \\ 1+\exp(ik) & 0 & 1+\exp(-ik) & & & \\ & 1+\exp(ik) & \cdot & \cdot & & \\ & & \cdot & \cdot & & \\ & & & 1+\exp(ik) & 0 & 1+\exp(-ik) \\ & & & & 1+\exp(ik) & F \end{bmatrix},$$

$$F = (-1)^{\lambda} 2\cos(\tfrac{1}{2}k).$$

The state in which the down-spins are neighbors is associated with the first row and column. The state in which the down-spins are farthest apart is associated with the last. The origin of the bound states and

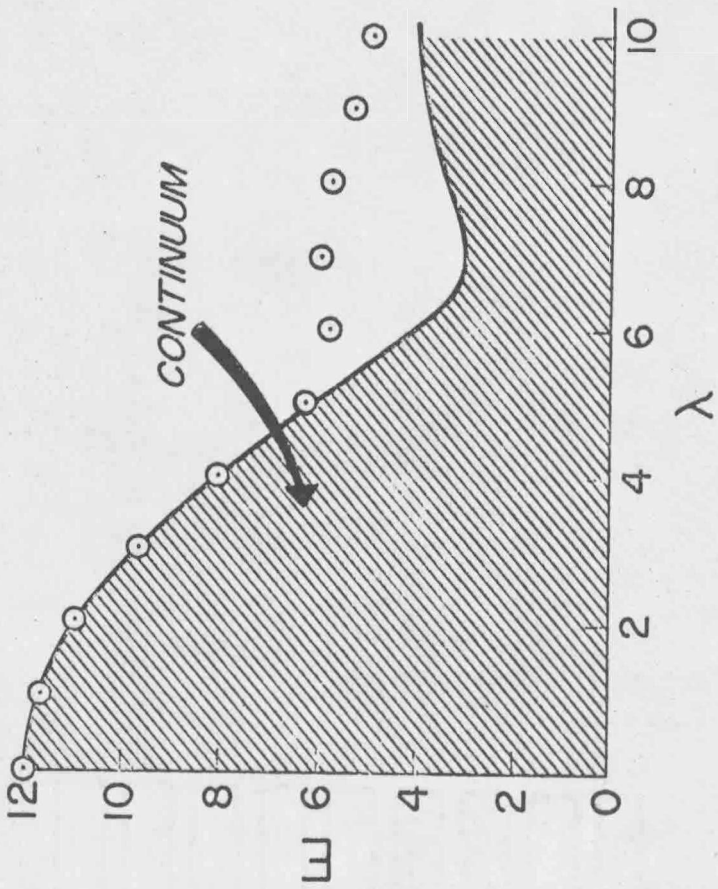


Fig. 9. The highest energy for states of the triangular lattice along $k=k_x=k_y$, $k=2\pi\lambda/n$ in this case n=21.

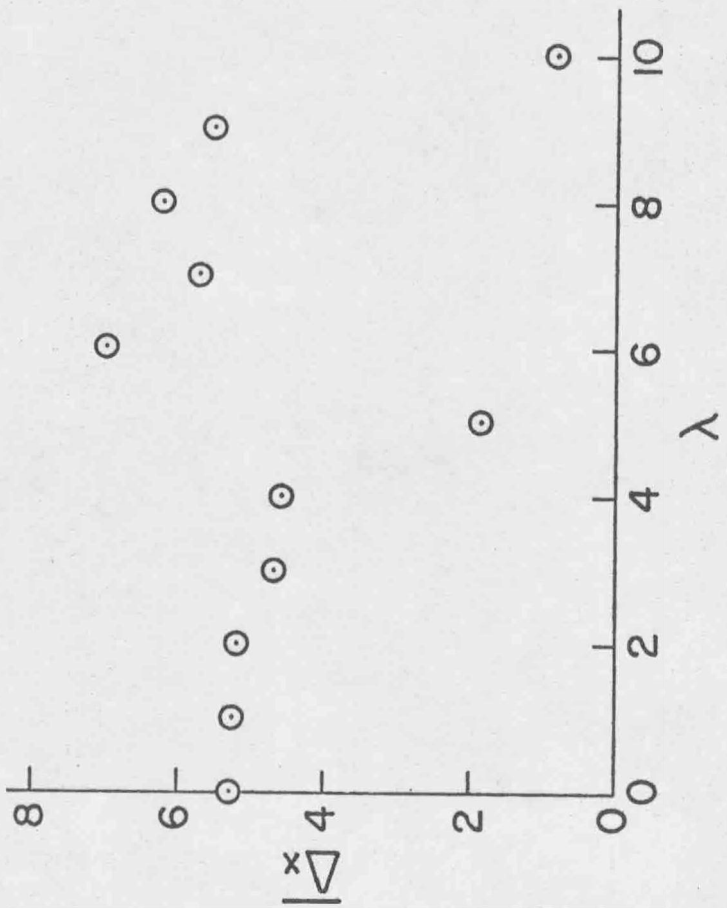


Fig. 10. Average separation in the x direction for the states shown in Fig. 9.

the attraction between the magnons lies in the 2 in the upper left-hand corner of H_1 as for $k \approx \pi$ all off-diagonal terms are small and in zeroth order perturbation theory 2 is an eigenvalue separated from a continuum of zeros which corresponds to a bound state. Consequently, the basis state in which the two down-spins are neighbors contributes the most to the bound state. As k approaches 0 the function F increases in magnitude until it obtains as much importance as the 2 in the upper left-hand corner. The F does the same thing, for the state in which the down-spins are as far apart as possible, as the 2 does for the state in which they are neighbors. F creates a force of repulsion between the two down-spins when it is positive just as the 2 creates an attractive force. In one dimension this repulsive force is never as strong as the attractive force. In two dimensions there is more opportunity for the two down-spins to be as far apart as possible in the x or y direction and it is therefore not surprising that the repulsive interaction is dominant.

The question remains whether this repulsion is important in the $N=\infty$ case. As was pointed out earlier, the independent spin-wave approximation is valid for the states of highest eigenvalue with small k, which is the region in which the repulsion is seen. By applying this approximation it was shown in one dimension that an oscillation of the average separations of the down-spins from one allowed value of k to the next remains even at $N=\infty$. A similar calculation for the two-dimensional square case shows that with $k_x=k_y=k$ there is no such oscillation as $k\to 0$

and that the separation of the two down-spins should be random for small k. This implies that the repulsive interaction is a finite size effect. In Figure 11, $\overline{\Delta x}/n$ is shown as a function of $1/n^2$ for the repulsive state of smallest k. It seems clear from this diagram that $\overline{\Delta x}$ approaches the random value from above and therefore for any finite n, regardless of how large, there is a slight repulsion between the magnons. Consequently, it is difficult to call this a bound state.

Conclusion and Discussion

Normally in systems that exhibit bound states there is a potential which is zero when the two particles are far apart. A bound state is any state having less than zero total energy. This definition does not fit the two magnon problem as there is no clearly defined potential. The magnons can be said to be bound when the energy of the state is different from the continuum energy and the down-spins tend to lie close together. If the magnon-magnon interaction is repulsive as it has been shown to be for some of the states whose energy lies outside the continuum, the states cannot be classed as bound. It seems that the eigenvectors as well as the eigenvalues must be investigated in order to classify states as bound or unbound. As can be seen in Figure 5 there is a sharp change in the eigenvectors for $k_x=k_y\approx\pi/2$. This could serve as a boundary between regions in which bound state behavior exists and does not exist.

The triangular lattice was investigated to determine only whether bound states were present and a bound state was found. The boundary

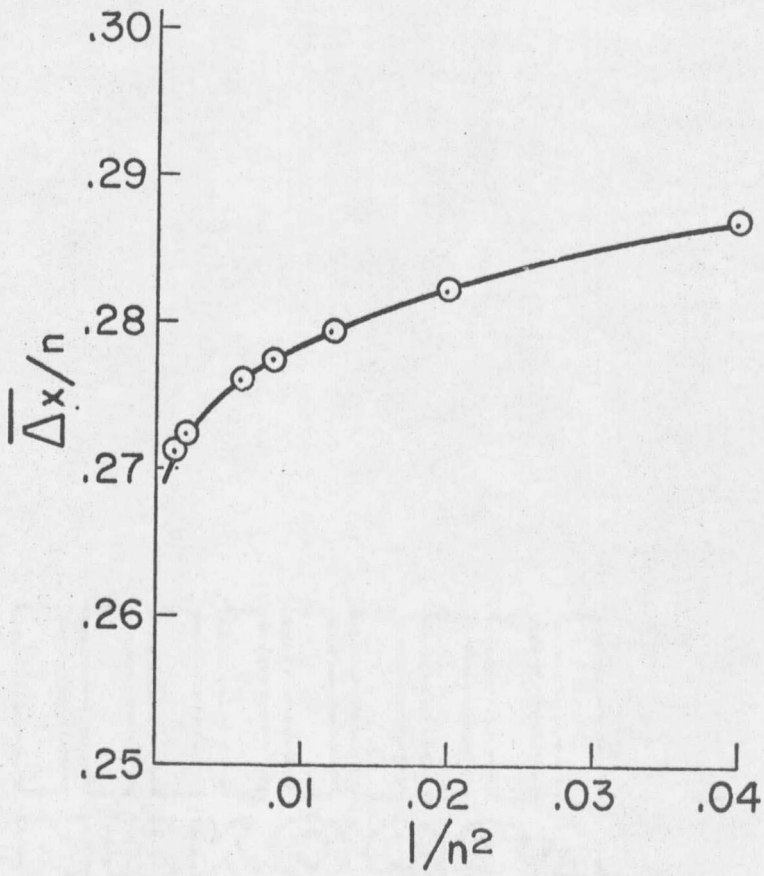


Fig. 11. Average separation in the x direction for the repulsive states of lowest $k=k_x=k_y$ as a function of $1/n^2$ showing the trend as $n>\infty$.

conditions used for the triangular lattice studied in this paper were chosen for the ease with which modifications could be made to the square lattice program. The boundary conditions chosen do not allow all of the symmetry operations normally associated with the triangular lattice. Certainly other boundary conditions could have been chosen. They are of great importance to the calculation of specific states even though they are not important when calculating thermodynamic properties. Therefore, as there seems to be no experimental or other interest in this problem for the triangular lattice, further details have not been carried out.

On the other hand the boundary conditions applied to the square lattice are natural ones to apply and there is other theoretical work with which to make comparison, notably the papers by Wortis [53] and Fukuda and Wortis [19], also, experimentally bound states have been shown to exist in one dimension [51] and quite good two-dimensional crystals with the square lattice are available [7, 9].

CHAPTER VI

CONCLUSION

A significant contribution that this thesis has attempted to make in the study of magnons is the development of small lattice techniques. In particular it should be easy to apply these techniques to three magnons in one dimension or to include next-nearest-neighbor interactions. Several applications of this technique have been presented here.

In one dimension the energies of all the states have been calculated, thus allowing approximations such as the hard sphere approximation to be tested.

Bound states in one dimension have been examined more extensively at small k in this thesis than previously in the work of Bethe, Flicker and Leff, Bonner and Fisher, or Oguchi. An approximation was made here that correctly predicted the behavior of all of the two-magnon states in this small k region. In the process of developing this approximation it was shown that the boson nature of spin-waves could be taken directly from the Hamiltonian. This has considerable pedagogic value. In addition, from the same approximation it was proved that bound states vanish in a class of lattices in one, two, and three dimensions at small k.

In two dimensions the behavior of the bound states was again examined. As was shown above the two down-spins seem to repel one another in two dimensions. The dependence of this repulsion on the boundary conditions was shown and it was further demonstrated that the

repulsive effect disappeared in the thermodynamic limit. It was shown, nevertheless, that the repulsive states exist for any finite periodic lattice and hence that these states cannot be considered bound. The definition of bound states for small k is a delicate one. The results above show that the energy based definition that was applied by Wortis and Bethe is not a good one. It is suggested that a better definition based on the wave functions should be developed, if indeed wave functions may be calculated for the infinite lattice. In light of this thesis such a redefinition is necessary.

As has been stated the value of recent studies of two-magnon states is not related to thermodynamics. The two-magnon problem is a study of solid state particles which have some similarities with, and many differences from, electrons and protons and are of interest for this reason. The bound state problem in particular has generated much theoretical and experimental effort as is mentioned above. For example Torrance and Tinkham have found bound states in Ising-like crystals ($CoCl_2 \cdot 2H_2O$). It would be of considerable difficulty, but of considerable interest, to discover them in more isotropic samples such as the $(NH_3)_2CuCl_4$ series, especially as only periodic boundary conditions have been applied in theoretical calculations and these are not physical. On the other hand, the non-periodic boundary condition problem is also one that would be interesting theoretically and one to which finite lattice calculations could be applied.

Other suggestions as to continuance of this work are the three-magnon problem in one dimension and the addition of next-nearest-

neighbor interactions as was previously stated. Theoretical work further exploring the analogies and differences between magnons and more usual physical particles would also be of interest.

APPENDICES

APPENDIX I

A calculation of the recursion relation for the characteristic equation for N_1 can be made as follows. Denote the determinant

$$\begin{vmatrix} -\lambda & 1+\exp(-ik) & & & \\ 1+\exp(ik) & -\lambda & 1+\exp(-ik) & & \\ & 1+\exp(ik) & . & . & \\ & & . & . & 1+\exp(-ik) \\ & & & 1+\exp(ik) & -\lambda \end{vmatrix}$$

with n rows and columns as $|n|$. Reducing by minors on the first row gives

$$|n| = -\lambda|n-1| - (2+2\cos k)|n-2|,$$

further

$$|1| = -\lambda ,$$

$$|2| = \lambda^2 - (2+2\cos k).$$

Thus $|n|$ may be evaluated for any n. Similarly reducing the determinant $|H_1 - \lambda I|$ by minors gives

$$|H_1 - I| = (2-\lambda)(F-\lambda)|n-2| - (2+2\cos k)[(F-\lambda)+(2-\lambda)]|n-3| + (2+2\cos k)^2|n-4|,$$

where n is the number of rows and columns in H_1. By evaluating $|n|$ and substituting in the above the characteristic polynomial for H_1 may be

generated. The procedure is quite mechanical and the coefficients of the powers of λ may be evaluated by a computer.[1]

[1] See Appendix III.

APPENDIX II

As a clarifying example the ring with five sites will be worked out in detail. There are ten basis states $\xi(m_1,m_2)$:

x x o o o
o x x o o
o o x x o
o o o x x
x o o o x

x o x o o
o x o x o
o o x o x
x o o x o
o x o o x

where x marks the location of a down-spin. The basis which diagonalizes the rotation operator is then,

$$x\,x\,o\,o\,o + e^{ik}\,o\,x\,x\,o\,o + e^{2ik}\,o\,o\,x\,x\,o + e^{3ik}\,o\,o\,o\,x\,x + e^{4ik}\,x\,o\,o\,o\,x,$$

$$x\,o\,x\,o\,o + e^{ik}\,o\,x\,o\,x\,o + e^{2ik}\,o\,o\,x\,o\,x + e^{3ik}\,x\,o\,o\,x\,o + e^{4ik}\,o\,x\,o\,o\,x,$$

where k may have any of its five allowed values.

Application of all possible nearest neighbor permutations to the first state gives,

$$\text{Permute } 1,2 \begin{cases} x\,x\,o\,o\,o + e^{ik}\,x\,o\,x\,o\,o + e^{2ik}\,o\,o\,x\,x\,o + e^{3ik}\,o\,o\,o\,x\,x \\ + e^{4ik}\,o\,x\,o\,o\,x \end{cases}$$

Permute

$$2,3\begin{cases}+ x\,o\,x\,o\,o + e^{ik}\,o\,x\,x\,o\,o + e^{2ik}\,o\,x\,o\,x\,o + e^{3ik}\,o\,o\,o\,x\,x \\ + e^{4ik}\,x\,o\,o\,o\,x\end{cases}$$

$$3,4\begin{cases}+ x\,x\,o\,o\,o + e^{ik}\,o\,x\,o\,x\,o + e^{2ik}\,o\,o\,x\,x\,o + e^{3ik}\,o\,o\,x\,o\,x \\ + e^{4ik}\,x\,o\,o\,o\,x\end{cases}$$

$$1,4\begin{cases}+ x\,x\,o\,o\,o + e^{ik}\,o\,x\,x\,o\,o + e^{2ik}\,o\,o\,x\,o\,x + e^{3ik}\,o\,o\,o\,x\,x \\ + e^{4ik}\,x\,o\,o\,o\,x\end{cases}$$

$$= 3(x\,x\,o\,o\,o + e^{ik}\,o\,x\,x\,o\,o + e^{2ik}\,o\,o\,x\,x\,o + e^{3ik}\,o\,o\,o\,x\,x + e^{4ik}\,x\,o\,o\,o\,x)$$

$$+ (1 + e^{ik})(x\,o\,x\,o\,o + e^{ik}\,o\,x\,o\,x\,o + e^{2ik}\,o\,o\,x\,o\,x + e^{3ik}\,x\,o\,o\,x\,o + e^{4ik}\,o\,x\,o\,o\,x).$$

A similar calculation may be made for the other basis vector

$$x\,o\,x\,o\,o + e^{ik}\,o\,x\,x\,o\,o + e^{2ik}\,o\,o\,x\,x\,o + e^{3ik}\,x\,o\,o\,x\,o + e^{4ik}\,o\,x\,o\,o\,x$$

giving

$$(1 + e^{-ik})(x\,x\,o\,o\,o + e^{ik}\,o\,x\,x\,o\,o + e^{2ik}\,o\,o\,x\,x\,o + e^{3ik}\,o\,o\,o\,x\,x + e^{4ik}\,x\,o\,o\,o\,x)$$

$$+ [1 + (-1)^{\lambda} 2\cos(\tfrac{1}{2}k)](x\,o\,x\,o\,o + e^{ik}\,o\,x\,o\,x\,o + e^{2ik}\,o\,o\,x\,o\,x + e^{3ik}\,x\,o\,o\,x\,o + e^{4ik}\,o\,x\,o\,o\,x).$$

The matrix elements $\langle \phi_1 | H_1 | \phi_2 \rangle$, ϕ being a basis vector, may be found when the action of the Hamiltonian on the basis vectors is known, thus allowing the Hamiltonian to be written in matrix form. For the ring of

five spins H_1 is the sum of all nearest neighbor permutations minus an identity operator and H_1 may be written as

$$\begin{pmatrix} 2 & 1+e^{-ik} \\ 1+e^{ik} & -(1)^{\lambda}2\cos(\tfrac{1}{2}k) \end{pmatrix}$$

Similary for the ring of four spins there are six basis states $\xi(m_1,m_2)$

x x o o
o x x o
o o x x
x o o x

x o x o
o x o x

The basis which diagonalizes the rotation operator is then

$$x\ x\ o\ o + e^{ik}\ o\ x\ x\ o + e^{2ik}\ o\ o\ x\ x + e^{3ik}\ x\ o\ o\ x,$$

$$x\ o\ x\ o + e^{ik}\ o\ x\ o\ x + e^{2ik}\ x\ o\ x\ o + e^{3ik}\ o\ x\ o\ x$$

but $e^{2ik} = e^{i\pi\lambda} = (-1)^{\lambda}$. If $e^{2ik} = -1$ the basis state starting with x o x o vanishes leaving the normalized basis set

$$1/2(x\ x\ o\ o + e^{ik}\ o\ x\ x\ o + e^{2ik}\ o\ o\ x\ x + e^{3ik}\ x\ o\ o\ x)$$

$$1/\sqrt{2}(x\ o\ x\ o + e^{ik}\ o\ x\ o\ x),$$

if λ is even,

$$1/2(x\ x\ o\ o + e^{ik}\ o\ x\ x\ o + e^{2ik}\ o\ o\ x\ x + e^{3ik}\ x\ o\ o\ x)$$

if λ is odd. The matrix form of H_1 becomes

$$\begin{pmatrix} 2 & \sqrt{2}(1 + e^{-ik}) \\ \sqrt{2}(1 + e^{ik}) & 0 \end{pmatrix} \quad \lambda \text{ even},$$

$$(2) \qquad \lambda \text{ odd}.$$

APPENDIX III

```
C ********
C
C  PROGRAM TO FIND TWO-MAGNON EIGENVALUES FOR THE ONE-
C   DIMENSIONAL HEISENBERG FERROMAGNET.
C
C  METHOD: THE CHARACTERISTIC POLYNOMIAL IS GENERATED
C   FROM A RECURSIVE FORMULA AND A SEARCH IS MADE FOR
C   ZEROS.  ZEROS ARE OBTAINED BY NEWTON'S METHOD.
C
C  OUTPUT: OUTPUT IS TO A CAL-COMP PLOTTER THROUGH
C   A SUBROUTINE PACKAGE.  EIGENVALUES ARE PLOTTED AS
C   A FUNCTION OF TOTAL MOMENTUM TOGETHER WITH THE
C   ENERGIES OBTAINED FROM SIMPLE SPIN-WAVE THEORY.
C   VERTICAL AXIS FROM 4 TO -4,HORIZONTAL AXIS FROM 0
C   TO 2PI.
C
C ********
C
      DIMENSION P(1000,4),L(3),ITITLE(10)
      READ(105,1000) ITITLE
 1000 FORMAT(10A4)
      DO 99 N=11,31,10
C
C  SET UP RECURSIVE SWITCH
      DO 1 I=1,2
    1 L(I)=I+1
      L(3)=1
C
C  INITIATE PLOT
      CALL INIT(2.*3.1415927,0.,4.,-4.,0,ITITLE)
      DO 10 M=0,N
      M0=3
      M1=2
      M2=1
C
C  OBTAIN CHARACTERISTIC POLYNOMIAL
      DO 2 I=1,100
      DO 2 II=1,4
    2 P(I,II)=0.
      W=2.*3.1415927*(FLOAT(M)/FLOAT(N))
```

```
      F1=2.*(1.+COS(W))
      P(5,2)=-1.
      P(6,3)=1.
      P(4,3)=-F1
      DO 4 I=3,(N-5)/2
C
C  RECURSIVE SWITCH
      M2=M1
      M1=M0
      M0=L(M0)
      DO 3 II=4,I+4
      P(II,M0)=-P(II-1,M1)-F1*P(II,M2)
    3 CONTINUE
    4 CONTINUE
 1001 FORMAT(1X)
      F2=2.*COS(.5*W*(N+1))
      DO 5 I=4,(N+7)/2
      P(I,4)=P(I-2,M0)-(F2+2.)*P(I-1,M0)+2.*F2*P(I,M0)
     A+2.*F1*P(I-1,M1)-(2.+F2)*F1*P(I,M1)+F1*F1*P(I,M2)
    5 CONTINUE
      DO 6 I=4,(N+5)/2
      P(I,1)=FLOAT(I-3)*P(I+1,4)
    6 CONTINUE
C
C  SEARCH FOR ZEROS
      Y2=1.
      DO 62 K=1,100*N+1
      X=8.*FLOAT(K)/FLOAT(100.*N)-4.
      Y=0.
      DO 61 KK=4,(N+7)/2
      KKK=(N-1)/2-KK+8
   61 Y=Y*X+P(KKK,4)
C
C  IF ZERO IS FOUND GO TO 63
      IF(Y2*Y.LT.0.) GO TO 63
      Y2=Y
  615 CONTINUE
   62 CONTINUE
   10 CONTINUE
C
```

```
C  PLOT SPIN-WAVES
      DO 99 K1=-(N-1)/2,(N-1)/2
      T1=2.*3.1415927*FLOAT(K1)/FLOAT((N-1)/2)
      Y=4.*COS(T1)
      T2=.02*3.1415927
      CALL PLOT(XC(0.),YC(Y),3)
      Y=2.*(COS(T1+T2)+COS(T1))
      CALL PLOT(XC(T2),YC(Y),2)
      DO 99 K2=2,100
      X=FLOAT(K2)*T2
      Y=2.*(COS(T1+X)+COS(T1))
      CALL PLOT(XC(X),YC(Y),1)
   99 CONTINUE
      CALL PLOT(11.,0.,-3)
      STOP
   63 E=X
      Y2=-Y2
      DO 8 J=1,50
C
C  NEWTON'S METHOD
      Y1=0.
      Y=0.
      DO 7 I=4,(N+7)/2
      II=(N-1)/2-I+8
      Y=Y*X+P(II,4)
      Y1=Y1*X+P(II,1)
    7 CONTINUE
      X1=X-Y/Y1
      IF(ABS((X1-X)/X).LT..00005) GO TO 9
      X=X1
    8 CONTINUE
      WRITE(108,1002) E,X,M
 1002 FORMAT(1X,2F10.4,I5,'*')
      GO TO 95
    9 CALL PLUS(XC(W),YC(X),.1)
   95 GOT O 615
      END
```

```
      SUBROUTINE INIT(XMAX,XMIN,YMAX,YMIN,ISTYLE,ITITLE)
C
C ********
C
C  DRAWS AXES AND GRID FOR A GRAPH ON 8.5X11 INCH SECTION
C  OF PAPER.  THE SUBROUTINE WILL DRAW A NEW SET OF
C  AXES EACH TIME IT IS CALLED AND WILL MAKE MAXIMUM
C  USE OF CHART PAPER.
C
C  XMAX,XMIN,YMAX,YMIN ARE THE MAXIMA AND MINIMA
C  OF THE VARIABLES TO BE GRAPHED.
C
C  ISTYLE SELECTS THE POSITION OF THE AXES.
C
C  0 = NO AXES.
C  1 PLACES THE AXES IN THE LOWER LEFT CORNER.
C  2 PLACES THE X AXIS AT X=0.
C  3 PLACES THE AXES THROUGH (0,0).
C
C  ITITLE IS A 10 WORD (40 CHARACTER) LITERAL STRING
C  WHICH WILL BE PRINTED AT THE TOP OF THE GRAPH.
C
C  OUTPUT ALSO INCLUDES A PRINTED TABLE OF THE NUM-
C  ERICAL VALUES ASSOCIATED WITH THE GRID DRAWN.
C
C ********
C
      COMMON Y0,XMX,XMN,YMX,YMN
      DIMENSION ITITLE(10),FCT(2),D(2)
      DIMENSION NAME(2)
      DATA NAME/'REKLIS  '/
      DATA N/-1/
      XMX=XMAX
      XMN=XMIN
      YMX=YMAX
      YMN=YMIN
      D(1)=XMX-XMN
      D(2)=YMX-YMN
      IF(D(1).LE.0..OR.D(2).LE.0.) STOP
      IF(N.NE.-1) GO TO 1
```

```
      CALL SYMBOL(0.,0.,.25,NAME,90.,8)
      CALLPLOT(1.,0.,-3)
      CALL PLOT(0.,29.,2)
      CALL PLOT(0.,0.,1)
      N=0
      GO TO 2
    1 IF(N.NE.0) GO TO 4
      CALL PLOT(11.,0.,-3)
    2 CALL PLOT(11.,0.,3)
      CALL PLOT(0.,0.,2)
      CALL PLOT(11.,0.,1)
      CALL PLOT(11.,8.5,1)
      DX=8.5
      DO 3 I=1,3
      Y=FLOAT(I)*8.5
      CALL PLOT(11.,Y,1)
      CALL PLOT(0.,Y,1)
    3 CALL PLOT(11.,Y,1)
      CALL PLOT (11.,0.,1)
    4 Y0=FLOAT(N)*8.5
      N=N+1
      IF(N.GE.3) N=0
      IF(ISTYLE.EQ.0) GO TO 15
      DO 7 I=1,2
      FCT(I)=1.
    5 IF(FCT(I)*D(I).GE.10.) GO TO 6
      FCT(I)=FCT(I)*10.
      GO TO 5
    6 IF(FCT(I)*D(I).LT.100.) GO TO 7
      FCT(I)=FCT(I)/10.
      GO TO 6
    7 CONTINUE
      WRITE(108,1000) ITITLE
 1000 FORMAT(15X,10A4/5X,'VALUES ALONG AXIS AT COORDINATES A
     15X,'X',14X,'Y')
      GO TO (8,9,10),ISTYLE
    8 XA=XC(XMN)
      YA=YC(YMN)
      GO TO 11
    9 XA=XC(XMN)
```

```
      YA=YC(0.)
      GO TO 11
   10 XA=XC(0.)
      YA=YC(0.)
   11 CALL PLOT(XA,YA,3)
      CALL PLOT(XA,YC(YMX),2)
      CALL PLOT(XA,YC(YMN),1)
      CALL PLOT(XA,YA,1)
      CALL PLOT(XC(XMX),YA,1)
      CALL PLOT(XC(XMN),YA,1)
      CALL PLOT(XA,YA,1)
      X=FLOAT(INT(FCT(1)*XMX))/FCT(1)+1./FCT(1)
   12 X=X-1./FCT(1)
      IF(X.LT.XMN) GO TO 13
      CALL PLUS(XC(X),YA,.1)
      WRITE(108,1001) X
 1001 FORMAT(5X,E10.3)
      GO TO 12
   13 Y=FLOAT(INT(FCT(2)*YMX))/FCT(2)+1./FCT(2)
   14 Y=Y-1./FCT(2)
      IF(Y.LT.YMN) GO TO 15
      CALL PLUS(XA,YC(Y),.1)
      WRITE(108,1002)Y
 1002 FORMAT(20X,E10.3)
      GO TO 14
   15 CALL SYMBOL(.25,Y0+8.1,.25,ITITLE,0.,40)
      RETURN
      END



      FUNCTION XC(X)
C
C ********
C
C  FUNCTIONS XC AND YC CONVERT DATA FOR USE WITH INIT
C  AND SHOULD BE USED AFTER INIT HAS BEEN CALLED.  A
C  SAMPLE OF THEIR USE IS:
C     CALL PLUS(XC(1.),YC(1.),.25)
```

```
C  THIS CALL WILL DRAW A "+" AT COORDINATES (1.,1.)
C  ON THE GRAPH LAST SET UP BY INIT.
C
C ********
C
      COMMON Y0,XMX,XMN,YMX,YMN
      XC=(X-XMN)*(7./(XMX-XMN))+2.5
      IF(X.LT.XMN) XC=2.4
      IF(X.GT.XMX) XC=9.6
      RETURN
      END


      FUNCTION YC(Y)
      COMMON Y0,XMX,XMN,YMX,YMN
      YC=(Y-YMN)*(5./(YMX-YMN))+Y0+2.
      IF(Y.LT.YMN)YC=Y0+1.9
      IF(Y.GT.YMX) YC=Y0+7.1
      RETURN
      END



      SUBROUTINE PLUS(X,Y,H)
C
C ********
C
C  DRAWS A "+" CENTERED AT PLOTTER COORDINATES X,Y
C  (INCHES) H INCHES HIGH.
C
C ********
C
      CALL PLOT(X,Y,3)
      CALL PLOT(X+H/2,Y,2)
      CALL PLOT(X-H/2,Y,1)
      CALL PLOT(X,Y,1)
      CALL PLOT(X,Y+H/2,1)
      CALL PLOT(X,Y-H/2,1)
      CALL PLOT(X,Y,1)
```

```
RETURN
END
```

APPENDIX IV

It is of importance to two-dimensional calculation to be able to determine which diagrams are equivalent. There is a procedure that may be used to do this. In one dimension

x o x o o

is equivalent to

x o o x o,

as in each case the down-spins are separated by one up-spin. In order to find the diagram equivalent to

x o x o o

one rotates the labeling until the down-spin that is not at the end to the left lies at the end to the left. In two-dimensions rotations must be performed in two directions to bring the down-spin that is not at the lower left-hand corner to the corner, thus

o o o o o
o o o o o
o o o o o
o o o x o
x o o o o

is equivalent to

o o x o o
o o o o o
o o o o o
o o o o o
x o o o o .

The following rule was developed to obtain the equivalent pairs more easily. Place a point at the center of the lattice which remains after the bottom row and left column have been removed, giving

```
o | o o o o
o | o o.o o
o | o o o o
o | o o x o
  x o o o o .
```

Then project the down spin in the remaining diagram through the point, giving

```
o | o x o o
o | o o.o o
o | o o o o
o | o o o o
  x o o o o ,
```

which is the equivalent diagram. This rule also holds for the diagrams in which the down spins are in the same row or column, if the periodic boundary conditions are employed, thus

```
o o o o o
o o o.o o
o o o o o
o o o o o
x o x o o
```

is equivalent by the rule to

```
      x
o o o o o
o o o.o o
o o o o o
o o o o o
x o o o o ,
```

which is

o o o o o
o o o o o
o o o o o
o o o o o
x o o x o .

This rule leads directly to the construction of the region of non-equivalent sites for the down spin not at the corner, which was referred to in the text.

Two equivalent states represent two basis states which are proportional. The proportionality constant is dependent on k_x and k_y and is just the product of the rotation operators $e^{i(k_x+k_y)}$ which rotates the second down spin to the corner.

APPENDIX V

```
C ********
C
C  PROGRAM TO FIND TWO-MAGNON BOUNDSTATES IN TWO-
C  DIMENSIONAL HEISENBERG FERROMAGNETS.
C
C  METHOD: ITERATIVE, SEE C. GERALD APPLIED NUMERICAL
C  ANALYSIS (ADDISON-WESLEY, READING, MASS. 1970) PP.
C  182-183.
C
C  ALLOCATION: A DOUBLE ARRAY (A) OF BASISVECTOR COEF-
C  ICIENTS IS USED.  THIS IS SWITCHED SO THAT THE HAM-
C  ILTONIAN IS APPLIED TO ONE ARRAY; THE RESULT IS
C  PLACED IN THE SECOND.  THE HAMILTONIAN IS THEN AP-
C  PLIED TO THE RESULT.
C
C  OUTPUT: OUTPUT IS TO THE LINE PRINTER AND TO A FILE.
C  THE RECORD IS (ENERGY, AVE. X SEPARATION, AVE. Y SEP-
C  ARATION, LAMBDA X, LAMBDA Y, PARITY UNDER INTERCHANGE
C  OF X AND Y).
C
C ********
C
      IS(I)=I+2
      COMPLEX A(23,13,2),EP1,EP2,EM1,EM2,AS
      DIMENSION L(2)
      COMMON A,EP1,EP2,EM1,EM2,AK1,L
      COMMON LK,LKK,N
C
C  SET UP SWITCH
      L(1)=2
      L(2)=1
      P=3.1415927
      LK=1
      INPUT N
      D=.5E-10
C
C  CLEAR COEFFICIENT ARRAY
      DO 1 I=1,N+2
      DO 1 II=1,(N+5)/2
      DO 1 III=1,2
```

```
    1 A(I,II,III)=(0.,0.)
C
C   BOUNDSTATE TRIAL SOLUTION
      A(IS(0),IS(1),LK)=(1.,0.)
      A(IS(N),IS(1),LK)=(1.,0.)
C
C   PICK LAMBDAS
      DO 12 L2=(N-1)/2,0,-1
      L1=L2
      AK1=2.*P*FLOAT(L1)/FLOAT(N)
      AK2=2.*P*FLOAT(L2)/FLOAT(N)
      EM1=(1.,0.)+CEXP(-CMPLX(0.,AK1))
      EM2=(1.,0.)+CEXP(-CMPLX(0.,AK2))
      EP1=(1.,0.)+CEXP(CMPLX(0.,AK1))
      EP2=(1.,0.)+CEXP(CMPLX(0.,AK2))
      SN=0.
C
C   TRY FOR CONVERGENCE 1500 TIMES
      DO 8 J=1,1500
C
C   SWITCH COEFFICIENT ARRAY
      LKK=LK
      LK=L(LK)
C
C   APPLY HAMILTONIAN
      DO 2 I=0,N-1
      DO 2 II=0,(N-1)/2
    2 A(IS(I),IS(II),LK)=EP1*A(IS(I-1),IS(II),LKK)
     A+EM1*A(IS(I+1),IS(II),LKK)
     B+EP2*A(IS(I),IS(II-1),LKK)
     C+EM2*A(IS(I),IS(II+1),LKK)
C
C   SUBROUTINE INSERTED TO MAKE THE COMPUTER HAPPY
      CALLSUB
C
C   ENFORCE BOUNDARY CONDITIONS
      DO 3 II=0,(N-1)/2
      A(IS(-1),IS(II),LK)=A(IS(N-1),IS(II),LK)
      A(IS(N),IS(II),LK)=A(IS(0),IS(II),LK)
    3 CONTINUE
```

```
      DO 4 I=0,N-1
C
C  EFFICIENCY
      A(IS(I),IS(-1),LK)=A(IS(N-I),IS(1),LK)
     A*CEXP(CMPLX(0.,AK1*FLOAT(I)-AK2))
      A(IS(I),IS((N+1)/2),LK)=A(IS(N-I),IS((N-1)/2),LK)
     A*CEXP(CMPLX(0.,AK1*FLOAT(I)+AK2*FLOAT((N+1)/2)))
    4 CONTINUE
C
C  RENORMALIZE
      S=0.
      DO 5 I=0,N-1
      DO 5 II=1,(N-1)/2
      SS=CABS(A(IS(I),IS(II),LK))
      SS=SS*SS
      S=S+SS
    5 CONTINUE
      DO 6 I=1,(N-1)/2
      SS=CABS(A(IS(I),IS(0),LK))
      SS=SS*SS
      S=S+SS
    6 CONTINUE
C
C  S IS THE EIGENVALUE
      S=SQRT(S)
      AS=CMPLX(1./S,0.)
      DO 7 I=1,N+2
      DO 7 II=1,(N+5)/2
    7 A(I,II,LK)=A(I,II,LK)*AS
C
C  HAS S CONVERGED?
      IF(ABS((S-SN)/S).LT.D) GO TO 9
      SN=S
    8 CONTINUE
C
C  TRIED 1500 TIMES AND HAS NOT COMVERGED
      WRITE(108,1001)
 1001 FORMAT(1X,'*')
    9 CONTINUE
C
```

```
C  CALCULATE RADIUS
      R=0.
      RX=0.
      RY=0.
      DO 10 I=1,(N-1)/2
      DO 10 II=0,(N-1)/2
      SS=CABS(A(IS(I),IS(II),LK))
      SS=SS*SS
      RRX=SS*FLOAT(I)
      RRY=SS*FLOAT(II)
      RX=RX+RRX
      RY=RY+RRY
      R=R+RRX+RRY
   10 CONTINUE
      DO 11 I=(N+1)/2,N
      DO 11 II=1,(N-1)/2
      SS=CABS(A(IS(I),IS(II),LK))
      SS=SS*SS
      RRX=SS*FLOAT(N-I)
      RRY=SS*FLOAT(II)
      RX=RX+RRX
      RY=RY+RRY
      R=R+RRX+RRY
   11 CONTINUE
      PAR=REAL(A(IS(1),IS(0),LK)/A(IS(0),IS(1),LK))
      WRITE(108,1002) S,RX,RY,R,L1,L2,PAR
      WRITE(  1,1002) S,RX,RY,R,L1,L2,PAR
 1002 FORMAT(1X,4F10.4,2I5,F10.4)
   12 CONTINUE
      CALL EXIT
      END
```

```
      SUBROUTINE SUB
      IS(I)=I+2
      DIMENSION L(2)
      COMPLEX A(23,13,2),EP1,EP2,EM1,EM2
      COMMON A,EP1,EP2,EM1,EM2,AK1,L
      COMMON LK,LKK,N
      A(IS(0),IS(1),LK)=(2.,0.)*A(IS(0),IS(1),LKK)
     A+EM2*A(IS(0),IS(2),LKK)
     B+EM1*A(IS(1),IS(1),LKK)
     C+EP1*A(IS(-1),IS(1),LKK)
      A(IS(1),IS(0),LK)=(2.,0.)*A(IS(1),IS(0),LKK)
     A+EM1*A(IS(2),IS(0),LKK)
     B+EM2*A(IS(1),IS(1),LKK)
     C+EP2*A(IS(1),IS(-1),LKK)
      A(IS(N-1),IS(0),LK)=A(IS(1),IS(0),LK)
     A*CEXP(CMPLX(0.,-AK1))
      RETURN
      END
```

BIBLIOGRAPHY

1. Baxter, R. J. One Dimensional Anisotropic Heisenberg Chain. Phys. Rev. Letters 26, 834 (1971).

2. Bethe, H. Zur Theorie der Metalle, I. Eigenwerte und Eigenfunktion der Linearen Atomkette. Z. Physik 71, 205 (1931).

3. Bloch, F. Zur Theorie des Feromagnetismus. Z. Physik 61, 206 (1930).

4. Boyd, R. G. and Joseph Callaway. Spin-Wave Spin-Wave Scattering in a Heisenberg Ferromagnet. Phys. Rev. A138, 1621 (1965).

5. Bonner, Jill C. and Michael I. Fisher. Linear Magnetic Chains with Anisotropic Coupling. Phys. Rev. A135, 640 (1964).

6. Bulaevskii, L. N. Theory of a Linear Anti-Ferromagnetic Chain. Sov. Phys.-JETP 16, 685 (1963).

7. de Jongh, L. J. Critical Behavior of the Perpendicular Susceptibility of Antiferromagnetic $(C_2H_5 NH_3)_2CuCl_4$. Solid State Com. 10, 537 (1972).

8. des Cloizeaux, Jacques and J. J. Pearson. Spin-Wave Spectrum of the AntiFerromagnetic Linear Chain. Phys. Rev. 128, 2131 (1962).

9. Drumheller, John E., D. H. Dickey, R. P. Reklis, C. E. Zaspel and Solomon T. Glass. Exchange Energy Constants in Some $S=\frac{1}{2}$ Two-Dimensional Heisenberg Ferromagnets. Phys. Rev. B5, 4631 (1972).

10. Dyson, Freman J. General Theory of Spin-Wave Interactions. Phys. Rev. 102, 1217 (1956).

11. _____. Thermodynamic Behavior of an Ideal Ferromagnet. Phys. Rev. 102, 1230 (1956).

12. Elliot, R. J., M. F. Thorpe, G. F. Insbusch, R. Louden and J. B. Parkinson. Magnon-Magnon and Exiton-Magnon Interaction Effects on AntiFerromagnetic Spectra. Phys. Rev. Letters 21, 147 (1968).

13. Faddeev, L. D. Scattering Theory for a Three-Particle System. Sov. Phys.-JETP 12, 1014 (1961).

14. Fleury, P. A. Evidence for Magnon Interactions in $RbMnF_3$. Phys. Rev. Letters 21, 151 (1968).

15. Flicker, Michael and Harvey S. Leff. On the Bethe Hypothesis for the Anisotropic Heisenberg Chain. Phys. Rev. 168, 578 (1968).

16. Fogedby, Hans C. Interacting Magnons in the Linear Chain. Phys. Rev. B5, 1941 (1972).

17. _____. The Intensity Spectrum of the Anisotropic Magnetic Chain. to be published.

18. Fogedby, Hans C. and Hojgaard Jensen. Energy Spectrum of the Anisotropic Magnetic Chain. Phys. Rev. B6, 3444 (1972).

19. Fukuda, Nobuyuki and Michael Wortis. Bound States in the Spin-Wave Problem. J. Phys. Chem. Solids 24, 1675 (1963).

20. Halley, J. Woods and I. Silvera. Odd Exiton-Magnon Interaction and Explanation of Anomalous Far-Infared Absorption in Anti-Ferromagnetic FeF_2. Phys. Rev. Letters 15, 654 (1965).

21. Hanus, Jean. Bound States in the Heisenberg Ferromagnet. Phys. Rev. Letters 11, 336 (1963).

22. Heisenberg, W. Zur Theorie des Ferromagnetismus. Z. Physik. 49, 619 (1928).

23. Huber, D. L. Distribution of Magnon Modes in a Disordered Magnetic Chain. Brookhaven National Laboratory Bul. BNL17480.

24. Hulthen, L. Arkiv. Mat. Astron. Fysik. A26, 1 (1938).

25. Johnson, James D. and Barry M McCoy. Low Temperature Thermodynamics of the $|\Delta| \leq 1$ Heisenberg-Ising Ring. Phys. Rev. A4, 1613 (1972).

26. Katsara, Shigetoshi. Two Body Problem in the One-Dimensional Heisenberg Model. Ann. Phys. (N.Y.) 31, 325 (1965).

27. Lovesey, S. W. and E. Balcar. Bound States in Heisenberg Anti-Ferromagnets. Phys. Letters 30A, 84 (1969).

28. Lovesey, S. W. and R. A. Meserve. Dynamic Properties of a One-Dimensional Heisenberg Magnet. Phys. Rev. Letters 28, 614 (1972).

29. Majumdar, Chanchal K. Application of the Faddeev Method to the Three-Spin Deviation Problem for the Heisenberg Model. Phys. Rev. B1, 287 (1970).

30. _____. Problem of Two Spin Deviations in a Linear Chain with Next-Nearest-Neighbor Interactions. J. Math Phys. 10, 177 (1969).

31. Mermin, N. O. and H. Wagner. Absence of Ferromagnetism or Anti-Ferromagnetism in One- or Two-Dimensional Isotropic Heisenberg Models. Phys. Rev. Letters 17, 1133 (1966).

32. Mubayi, V., K. Krishan and C. K. Majumdar. Heisenberg Model for the 3x3 Square Lattice. J. Phys. Soc. Japan 34, 1153 (1973).

33. Ngai, K. L., J. Ruvalds and E. N. Economou. Bound Magnon Pairs in Metamagnetic Systems. Phys. Rev. Letters 31, 166 (1973).

34. Oguchi, Takehiko. Theory of Two Magnon Bound States in the Heisenberg Ferro- and Antiferromagnet. J. Phys. Soc. Japan 31, 394 (1971).

35. _____. Theory of Two-Magnon Bound States in a Two-Dimensional Antiferromagnet. J. Phys. Soc. Japan 31, 394 (1971).

36. Ono, Ikuo, Syogo Mikado and Takehiko Oguchi. Two-Magnon Bound States in a Linear Heisenberg Chain with Nearest and Next Nearest Neighbor Interactions. J. Phys. Soc. Japan 30, 358 (1971).

37. Ovchinnikov, A. A. Complexes of Several Spins in a Linear Heisenberg Chain. JETP Letters 5, 38 (1967).

38. _____. Excitation Spectrum of an Antiferromagnetic Heisenberg Chain. Sov. Phys.-JETP. 29, 727 (1969).

39. Reklis, R. P. Numerical Calculations of Two-Spin-Wave Bound States in Some Two-Dimensional Heisenberg Ferromagnets. To be published.

40. Reklis, R. P. and John E. Drumheller. Numerical Calculation of Two-Spin-Wave States in the One-Dimensional Heisenberg Ferromagnet. Phys. Rev. To be published.

41. Richards, P. L. Far Infared Absorption by Two-Magnon Excitations in Antiferromagnets. J. Appl. Phys. 38, 1500 (1967).

42. Sa'enz, A. W. and W. W. Zachary. Two-Magnon Bound States in Heisenberg Ferromagnets. To be published.

43. Sharon, T. M. and A. A. Maradudin. Magnon Edge Modes. Solid State Comm. 13, 187 (1973).

44. Silberglitt, Richard and Jerry B. Torrance, Jr. Effect of Single Ion Anisotropy on Two-Spin-Wave Bound States in a Heisenberg Ferromagnet. Phys. Rev. B2, 772 (1970).

45. Stanley, H. E. and T. A. Caplan. Possibility of a Phase Transition for the Two-Dimensional Heisenberg Model. Phys. Rev. Letters 17, 913 (1966).

46. Sukiennicki, A. and A. Zagorski. On Anisotropic One-Dimensional Heisenberg Chain with Impurities. Phys. Letters 29A, 684 (1969).

47. Tonegawa, Takashi. Two-Magnon Bound States in the Heisenberg Ferromagnet with Anisotropic Exchange and Unaxial Anisotropy Energies. Supplement of Prog. Theor. Phys. 46, 61 (1970).

48. Thorpe, M. F. Two-Magnon Bound States in fcc Ferromagnets. Phys. Rev. B5, 1608 (1971).

49. Torrance, J. B. Jr. and K. A. Hay. Simultaneous Excitation of a Magnon plus a Phonon in $CoBr_2 \cdot 2H_2O$: A New Type of Bound State? Phys. Rev. Letters 31, 163 (1973).

50. Torrance, J. B. Jr. and M. Tinkham. Far-Infared Absorption in $CoCl_2 \cdot 2H_2O$. J. Appl. Phys. 39, 822 (1968).

51. _____. Magnon Bound States in Anisotropic Linear Chains. Phys. Rev. 187, 587 (1969).

52. Weiss, P. J. Phys. Radium, Paris 6, 667 (1907).

53. Wortis, Michael. Bound States of Two Spin Waves in the Heisenberg Ferromagnet. Phys. Rev. 132, 85 (1963).

General References

54. Feynman, R. P. Statistical Mechanics—a Set of Lectures (W. A. Benjamin, Inc., Reading, Mass., 1972).

55. Gerald, Curtis F. Applied Numerical Analysis (Addison-Wesley, Reading, Mass., 1970).

56. Holstein, T. and H. Primakoff. Field Dependence of the Intriasic Domain Magnetization of a Ferromagnet. Phys. Rev. 58, 1098 (1940).

57. Huang, Kerson, Statistical Mechanics (Wiley, New York, 1963).

58. Keffer, Frederic. Spin Waves. Handbuch der Physik, 18, 1 (1966).

59. Stanley, H. Eugene. Introduction to Phase Transitions and Critical Phenomena (Oxford Univ. Press, New York, 1971).

60. Van Kranendonk, J. and J. H. Van Vleck. Spin Waves. Rev. Mod. Phys. 30, 1 (1958).

61. White, Robert M. Quantum Theory of Magnetism (McGraw-Hill, New York, 1970).