

type effects (i.e., an additional electron interacting with the electron line of the particle-hole ladder forming the dominant vertex). Although the characteristic " $f - \frac{1}{2}$ " effect is well known to occur in the numerators of such interaction terms,⁸ the summations over states seem to smooth out the associated logarithmic singularity. Thus, at this stage, we see no obvious way of

⁸ For example, in the considerations leading to the theory of superconductivity.

generating an s - d coupling with sharply singular properties of the Kondo type.

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Excitation Spectrum of Antiferromagnetic Rings

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Recently, Kawasaki proved that the biperiodicity of the dispersion relation obtained by des Cloizeaux and Pearson for the lowest triplet excitations of the Heisenberg antiferromagnetic ring is required by symmetry. This degeneracy is shown not to be a consequence of any symmetry of the Hamiltonian which has been noticed; it therefore appears to be accidental.

IN recent years, great interest has been attached to the properties of antiferromagnetic rings of Heisenberg-Ising coupled doublet sites. Such rings are described quantum mechanically by the Hamiltonian

$$\mathcal{H} = \sum_{n=1} \{ \gamma S_n^z S_{n+1}^z + (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) \},$$

$$S_{N+1} \equiv S_1. \quad (1)$$

Exact results have been obtained for the eigenstates,^{1,2} ground-state energy,³⁻⁵ short-range order,⁴ the ordering of energy levels,^{5,6} and the dispersion curve for low-lying collective excitations⁷ for $\gamma = 1$, which are triplets, using the arguments of Lieb and Mattis. Griffiths⁸ has obtained the magnetic susceptibility at absolute zero by considering the lowest eigenstates for given S^z values in the pure Heisenberg case. This has been extended with greater rigor by Yang and Yang⁹ to other values of γ ; these authors considered the equation of state at absolute zero.

The dispersion curve obtained by des Cloizeaux and Pearson⁷ is of the form

$$E(q, m) = \pi | \sin q | / 2, \quad e^{iqN} = +1, \quad m = 0, \pm 1. \quad (2)$$

This result was obtained in the limit $N \rightarrow \infty$; it is

curiously biperiodic; that is,

$$E(q) = E(q + \pi) = E(q + 2\pi). \quad (3)$$

A full statistical-mechanical analysis of the system has proved elusive, because an adequate general method of handling and classifying the eigenstates given by Bethe has not yet been found. Neither has the long-range order been evaluated in closed form, although Walker¹⁰ has given a perturbation expansion, and Mermin and Wagner¹¹ have proved that for the pure Heisenberg case there can be no long-range order. Bonner and Fisher¹² obtained exact results for finite rings using machine calculations.

For this reason, approximate methods¹³⁻¹⁷ have been developed using the Jordan-Wigner transformation of spin raising and lowering operators for doublets to Fermi site excitation creation and annihilation operators. These methods use further transformations which both exploit the inherent symmetry of (1) and which are canonical; the statistical mechanics is then, in principle, tractable.

Recently, Kawasaki¹⁸ claimed to have analyzed the symmetry properties of the Fermi representation for regular magnetic rings, and thereby to have proved the

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¹⁶ D. B. Abraham and A. D. McLachlan, Mol. Phys. **12**, 319 (1967).

¹⁷ S. Inawashiro and S. Katsura, Phys. Rev. **140**, A892 (1965).

¹⁸ K. Kawasaki, Phys. Rev. **142**, 164 (1966).

double periodicity in the triplet excitation spectrum to be required by symmetry.

In this paper, we shall disprove Kawasaki's theorem, thus demonstrating that the biperiodicity is an accidental degeneracy, in so far as it is not required by any symmetry noticed as yet; furthermore, this degeneracy appears asymptotically as $N \rightarrow \infty$ in the alternant spin-wave theory.¹⁶

KAWASAKI'S THEOREM

An analysis of the symmetry properties of (1) has been given by Abraham and McLachlan,¹⁹ whose ideas and notation we shall use. \mathcal{H} is invariant under the operations T^r of the one-dimensional translation group τ_N , and the operations of the double group of rotations about the z axis $\{E, R(z, \pi), R(z, 2\pi), R(z, 3\pi)\}$, or equivalently, the parity group $\{E, (-1)^\sigma\}$, where

$$\sigma = \sum_{n=1}^N (S_n^z + \frac{1}{2}).$$

Further, \mathcal{H} commutes with S^z , a stronger requirement than that above. Consequently, the eigenstates have the form

$$|q, m\rangle = \sum_n \Delta(\frac{1}{2}N + m - n) \sum_{k_1 \dots k_n} A(k_1 \dots k_n) \times \Delta(k_1 + \dots + k_n - q) F_{k_1}^\dagger \dots F_{k_n}^\dagger |0\rangle, \quad (4)$$

where

$$e^{ik_j N} = (-1)^{n-1}$$

and

$$\Delta(x) = 1, \quad x = 2r\pi, r = 0, \pm 1, \dots \\ = 0, \quad \text{otherwise.}$$

The F_k^\dagger are Fermi creation operators, defined by¹⁹

$$F_k^\dagger = N^{-1/2} \sum_{n=1}^N e^{ikn} \exp[i\pi \sum_{m=1}^{n-1} (S_m^z + \frac{1}{2})] S_n^\dagger.$$

The apparently bizarre restriction in Eq. (4) on the single-Fermion wave numbers is necessary for $F_{k_1}^\dagger \dots F_{k_n}^\dagger |0\rangle$ itself to be a symmetry state; Kawasaki did not realize this. Under these conditions, $|q, m\rangle$ has the properties

$$T|q, m\rangle = e^{iq} |q, m\rangle, \quad e^{iqN} = +1 \\ S^z |q, m\rangle = m |q, m\rangle, \quad m = 0, \pm 1, \dots, \pm \frac{1}{2}N. \quad (5)$$

Now suppose N is even; the ground state^{5,6} will have $m=0$ and will be of the form

$$|q_0, 0\rangle = \sum_{k_1 \dots k_{N/2}} \Delta(k_1 + \dots + k_{N/2} - q) \times A_0(k_1 \dots k_{N/2}) F_{k_1}^\dagger \dots F_{k_{N/2}}^\dagger |0\rangle, \quad (6)$$

with

$$e^{ik_j N} = (-1)^{[(N/2)+1]}.$$

The wave function $A_0(k_1 \dots k_{N/2})$ may be related to the Bethe ground state: $q_0 = (0, \pi)$ for $\frac{1}{2}N$ (even, odd). There is another state $|q_1, 0\rangle$ with wave function $A_1(k_1 \dots k_{N/2})$ and $q_1 = (\pi, 0)$ for $\frac{1}{2}N$ (even, odd) whose energy is asymptotically the same as that of $|q_0, 0\rangle$.

An excited state $|q_0 + q, m\rangle$ with excitation energy $E(q, m)$ may be obtained from the ground state by setting

$$|q_0 + q, m\rangle = W(q, m) |q_0, 0\rangle, \quad (7)$$

where the operator $W(q, m)$ may be written

$$W(q, m) = \sum_n \sum_{\{k\}} \sum_{\{\delta\}} A_m(k_1 \dots k_n) \Delta(\delta_1 + \dots + \delta_{n-m}) \times \Delta(k_1 \delta_1 + \dots + k_n \delta_{n-q}) F_{k_1}^{\delta_1} \dots F_{k_n}^{\delta_n}, \quad (8)$$

with

$$F_k^\delta = F_k^\dagger, \quad \delta = +1 \\ = F_k, \quad \delta = -1.$$

Now Kawasaki's theorem states that

$$E(q, m) = E(-q + \pi, -m) = E(q + \pi, -m), \\ m \text{ odd} \\ E(q, m) = E(-q, -m) = E(q, -m), \\ m \text{ even.} \quad (9)$$

The theorem for m odd is false; that for m even is true, but incorrectly proven. To see why this is so, we must investigate (8).

It is certainly true that $|q_0 + q, m\rangle$ may be written as in (7), but each operator $F_{k_1}^{\delta_1} \dots F_{k_n}^{\delta_n}$ does not necessarily span an irreducible representation of τ_N , which is contrary to Kawasaki's assumption. In this analysis, Abraham and McLachlan¹⁹ showed that operators may be classified according to the irreducible representation of $\{E, (-1)^\sigma\}$ which they span. Even symmetry operators $F_{k_1}^{\delta_1} \dots F_{k_{2n}}^{\delta_{2n}}$ will appear as

$$F_{\alpha_1}^{\delta_1} \dots F_{\alpha_{2n}}^{\delta_{2n}} Q(\alpha) + F_{\beta_1}^{\delta_1} \dots F_{\beta_{2n}}^{\delta_{2n}} Q(\beta), \quad (10)$$

where $e^{i\alpha N} = 1$, $e^{i\beta N} = -1$. $Q(\alpha)$ and $Q(\beta)$ are the projection operators for the even and odd irreducible representations of $\{E, (-1)^\sigma\}$. Notice that \mathcal{H} is an even operator:

$$\mathcal{H} = \mathcal{H}(\alpha) Q(\alpha) + \mathcal{H}(\beta) Q(\beta). \quad (11)$$

No simple Fermi representation is possible for odd symmetry operators; in particular, $F_{k_1}^{\delta_1} \dots F_{k_{2n+1}}^{\delta_{2n+1}}$ can never be a symmetry operator, no matter how the k is chosen.

In order to appreciate the consequences of this, we consider the transformation of $W(q, m)$ by time reversal u and rotation by π about the y axis, i.e., $R(y, \pi)$. It is clear that $W(q, m) \rightarrow W(q^\dagger, -m)$, in which $F_{k_1}^{\delta_1} \dots F_{k_n}^{\delta_n}$ is replaced by $F_{\pm k_1 + \pi}^{\delta_1} \dots F_{\pm k_n + \pi}^{\delta_n}$; the $+$ ($-$) sign obtains for $u(R)$. Thus

$$W(q, m) \rightarrow W(\mp q + \pi, -m), \quad m \text{ odd} \\ W(q, m) \rightarrow W(\mp q, -m), \quad m \text{ even.} \quad (12)$$

¹⁹ D. B. Abraham and A. D. McLachlan, Mol. Phys. **12**, 301 (1967).

When m is odd, $W(q, m)$ can never be a sum of terms in the Fermi representation, each of which is a symmetry operator on $|q_0, 0\rangle$, and so neither can be $XW(q, m)X^{-1}$, where $X=U$ or R . Consequently Kawasaki's assertion that $E(q, m)=E(\pm q+\pi, -m)$ for m odd is incorrect, because $|q_0, 0\rangle$ is nondegenerate,⁵ and is therefore transformed into itself by U and R . When m is even, $W(q, m)$ should take the form

$$W(q, m) = Q(\alpha)W_\alpha(q, m) + Q(\beta)W_\beta(q, m),$$

where

$$W_\alpha(q, m) = \sum_n \sum_{\{\alpha\}} \sum_{\{\delta\}} \Delta(\alpha_1\delta_1 + \cdots + \alpha_{2n}\delta_{2n} - q) \\ \times \Delta(\delta_1 + \cdots + \delta_{2n} - m) A_m(\alpha_1 \cdots \alpha_{2n}) F_{\alpha_1}^{\delta_1} \cdots F_{\alpha_{2n}}^{\delta_{2n}}, \quad (13)$$

with a similar form for W_β . Only in this form is $W(q, m)$ a sum of operators $F_{k_1}^{\delta_1} \cdots F_{k_n}^{\delta_n}$ each of which spans the irreducible representation $D^{(q)}(T^n) = e^{iqn}$ of τ_N . It is

then easy to show that Kawasaki's theorem for m even is correct, but the proof is false.

We now consider the effect of rotations $R(y, \pi)$, time reversal U , and reflections $R(S)$ on the state (q, m) , which has the properties of Eq. (5). These operations commute with \mathcal{H} and connect the states $|q, m\rangle$, $|q, -m\rangle$, $|-q, -m\rangle$, and $|-q, m\rangle$, which are consequently required to be degenerate. This is just what one would have expected; it proves that the states $|\pm q, \pm m\rangle$ and $|\pm q + \pi, \pm m\rangle$ are not connected by any symmetry of \mathcal{H} which has been considered, and consequently any degeneracy between them must be accidental. Nevertheless, such degeneracy can arise in a systematic way in the alternant spin-wave approximate theory of an antiferromagnetic ring¹⁹ for which $N \rightarrow \infty$.

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Magnetic Structures and Exchange Interactions in the Mn-Pt System

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The magnetic structures and transformations in the ordered phases of the Mn-Pt system have been investigated in a wide concentration range by magnetic, x-ray, and neutron diffraction methods. The properties of the $\text{Mn}_3\text{Pt}_{1-y}\text{Rh}_y$ and $\text{Mn}_{3-x}\text{Fe}_x\text{Pt}$ systems have also been studied. The triangular and the collinear antiferromagnetic structures, both found in the Mn_3Pt phase, undergo a first-order transformation into each other at a critical value of the lattice parameter where the next-nearest-neighbor interaction changes sign. In the MnPt phase a simple antiferromagnetic structure occurs with the directions of the magnetic moments dependent on concentration and temperature. There is no direct connection between the anisotropy energy and the lattice dimensions. The MnPt_3 phase has simple ferromagnetic structure. The measured transition temperatures are summarized in magnetic phase diagrams. The magnetic structures and transformations of the Mn-Pt system are explained by assuming nearest- and next-nearest-neighbor interactions dependent on the interatomic distances. The magnetic phase diagram of the Mn_3Pt phase calculated in the molecular-field approximation is in agreement with the experimental observations.

I. INTRODUCTION

THE metals of the $3d$ transition series form with platinum intermetallic compounds of ordered Cu_3Au and CuAu-I lattice type. These alloys show both antiferromagnetic and ferromagnetic behavior and their common feature is the existence of ordered magnetic moment on the Pt atoms in the ferromagnetic state.

In the Mn-Pt system, the ordered intermetallic compounds occupy a considerable part of the phase diagram obtained by Raub and Mahler¹ from x-ray diffraction and microscopic studies. At room temper-

ature the ordered Mn_3Pt , MnPt , and MnPt_3 phases are stable in the 16–29-at.% Pt, 33–60-at.% Pt, and 63–83-at.% Pt concentration ranges, respectively. According to the neutron diffraction measurements reported by Sidhu *et al.*,² in Mn_3Pt two antiferromagnetic structures, not specified in detail but having different Néel temperatures, coexist. The comparable compound Mn_3Rh has a noncollinear, triangular antiferromagnetic structure.³ The magnetic properties of

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