Ordering in Linear Antiferromagnetic Chains with Anisotropic Coupling

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Some reasonable conjectures are made concerning the finite-temperature pair correlations of spins with anisotropic antiferromagnetic coupling. These conjectures provide a general description of the ordering. Using them together with the finite value of the zero-temperature susceptibility, one obtains

$$S_1 < S_3 < \ldots < 0 < \ldots < S_4 < S_2,$$

where

$$S_n = 1 - (-1)^n \omega_\infty + 2 \sum_{l=1}^{n} \omega_l,$$

ω_l is the zero-temperature pair correlation, and ω_∞ is the infinite-l limit of $|\omega_l|$. Bonner and Fisher's finite-chain extrapolations for ω_l are in agreement with this result. Using their values of ω_l ($l=1,2,3,4,\infty$) and the inequality, bounds are computed for ω_5. The further conjecture that the rate of decrease in the absolute value of the correlation with distance is monotonic leads to a contradiction near the Heisenberg limit. The role of ω_∞ in the inequality and its derivation is particularly interesting since the limit $l \to \infty$ followed by $T \to 0$ of the pair correlation of spins separated by l-1 spins is probably zero and not ω_∞. When the correlations approximate their zero-temperature value out to a distance ξ such that $|\omega_\xi| \approx \omega_\infty$ and decrease slowly thereafter with increasing separation, then T_χ is approximately zero.

1. INTRODUCTION

Despite the simplicity usually associated with one-dimensional problems, the linear magnetic chain is in a sense more complicated than magnetic systems of higher dimensionality. The lack of long-range order at any finite temperature makes theories, such as spin-wave theory, which are based on deviations from an ordered state, inappropriate. Because of the absence of complete ordering at finite temperatures, the linear chain represents a favorable system for studying the increasing amount of short-range ordering that occurs with decreasing temperature.

The temperature dependence of the pair correlations is known only in the case of Ising coupling.[1] Falk[2] has shown that the absolute value of the nearest-neighbor correlations are nonincreasing functions of temperature for Heisenberg coupling. Because of the paucity of results for these correlations and their special relevance to this problem, it is reasonable to make some general conjectures concerning them in order to test their consequences and gain some insight into the manner in which the order increases with decreasing temperature. An answer will be suggested for the question, How does the finite-temperature order approach the zero-temperature order?

Bonner and Fisher[3] have used machine calculations on finite linear magnetic chains with anisotropic coupling to estimate the properties of infinite chains. In particular, for antiferromagnetic coupling they have estimated the zero-temperature pair correlation functions in zero external magnetic field defined by

$$\omega_l = 4 \lim_{N\to\infty} \frac{1}{N} \langle \sum_{j=1}^{N} S_j^Z S_{j+l}^Z \rangle, \quad T=0. \tag{1}$$

It should be noted that Orbach[4] has calculated ω_l exactly in the case of infinite N and Walker[5] has extended his work to find an expansion for ω_∞. The quantity ω_∞ is defined as the limit of $|\omega_l|$ for large l and has been used by several authors,[3,6] as a measure of the long-range order. It is thought that ω_∞ vanishes only for isotropic coupling.[3] The likelihood that $\omega_\infty \neq 0$ requires that special care be taken in estimating certain sums discussed below.

The Hamiltonian for a linear chain with anisotropic coupling is

$$\mathcal{H} = \mathcal{H}_E + \mathcal{H}_Z, \tag{2}$$

where

$$\mathcal{H}_E = -2J \sum_{i=1}^{N} [S_i^z S_{i+1}^z + \gamma (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)], \tag{3a}$$

$$\mathcal{H}_Z = -g\beta \sum_{i=1}^{N} S_i^z H, \quad J<0, \quad 0 \leq \gamma \leq 1, \tag{3b}$$

and the magnetic field H is in the Z direction. The treatment will be restricted to the case of spin $\frac{1}{2}$.

The zero-field susceptibility $\chi(T)$ will be related to the finite-temperature, infinite-chain, pair correlations. The limit $T \to 0$ such that $g\beta H \ll kT$ will be taken. One must first consider pair correlations at infinite separation before the limit $T \to 0$ is taken. Certain reasonable conjectures will be made concerning this double limiting process which provide a general description of the ordering. From these conjectures and the fact that $\chi(0) \neq \infty$

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[1] A. S. Edelstein, J. Chem. Phys. **40**, 488 (1964).

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[5] L. R. Walker, Phys. Rev. **116**, 1089 (1959).

[6] T. W. Ruijgrok and S. Rodriguez, Phys. Rev. **119**, 596 (1960).

a set of inequalities involving the ω_l's will be obtained. The special role played by the long range order ω_∞ in these inequalities and their derivation is significant. The long range order does not enter the problem in what would seem to be the most obvious way. One would expect the physically relevant quantity to have the limits taken in the opposite order. As will be discussed later, if the limit of infinite separation is taken before the limit $T\to 0$ then the result is probably zero and not ω_∞.

The fact that Bonner and Fisher's extrapolated values[3,7] of ω_l ($l=1, 2, 3, 4, \infty$) satisfy these inequalities supports the correctness of the conjectures. As an example of one use of these inequalities, they will be used in conjunction with the Bonner and Fisher values of ω_l to compute bounds on ω_5.

2. GENERAL FORMULATION AND CONJECTURES

The low-temperature limit of the zero-field susceptibility per particle,

$$\chi(T)=\lim_{H\to 0}\lim_{N\to\infty}\frac{kT}{N}\frac{\partial^2 F}{\partial H^2}, \tag{4}$$

where $F=\ln \mathrm{Tr}[e^{-\mathcal{H}/kT}]$ will be used to test a set of conjectures about the finite-temperature pair correlations. From the differentiation one obtains

$$4kT\chi(T)/(g\beta)^2=\lim_{N\to\infty}\frac{1}{N}\langle\sum_{i,j=1}^{N}\sigma_i\sigma_j\rangle - \lim_{H\to 0}\lim_{N\to\infty}\frac{1}{N}\left(\frac{2kT}{g\beta}\frac{\partial}{\partial H}F\right)^2, \tag{5}$$

where

$$\sigma_i=2S_i^z \tag{6}$$

and

$$\langle O\rangle=\mathrm{Tr}[Oe^{-\mathcal{H}_E/kT}]/\mathrm{Tr}[e^{-\mathcal{H}_E/kT}]. \tag{7}$$

The limit $H\to 0$ has been taken in the first term of Eq. (5) by considering a Taylor's series in the Zeeman Hamiltonian $\mathcal{H}_z$ for $g\beta|H|\ll kT$. Each term of the expansion is a product of a function of H and a function of N. Hence the $H\to 0$ limit can be taken before the limit $N\to\infty$ is taken.

The second term on the right of Eq. (5) is proportional to the square of the magnetization. In the limit $H\to 0$ it is certainly zero. There is no spontaneous magnetization in one dimension. Since the discussion is limited to antiferromagnetic coupling the magnetization would be zero even if there were spontaneous sublattice magnetizations since the sum of such magnetizations would be zero.

Hence[8]

$$4kT\chi(T)/(g\beta)^2=\lim_{N\to\infty}\frac{1}{N}\langle\sum_{i,j=1}^{N}\sigma_i\sigma_j\rangle. \tag{8}$$

[7] J. C. Bonner (private communication).

[8] M. E. Fisher [Phil. Mag. **7**, 1731 (1962)] has obtained an equation of nearly the same form as Eq. (8). The derivation has been repeated to emphasize that Eq. (8) is still valid for $kT\ll|J|$ provided that $g\beta|H|\ll kT$.

One might question the validity of Eq. (8) in the limit $T\to 0$. Walker[5] has shown that the point $\gamma=1$, $T=0$, $H=0$ is a special point since the ground state energy as a function of γ is nonanalytic at $\gamma=1$. Also, Griffiths' work[9] makes it highly likely that the magnetization is not analytic at this point. The limits $H\to 0$, $T\to 0$ will be taken such that $g\beta|H|\ll kT$. Hence the point $T=0$ is of necessity excluded. The pair correlations are defined by

$$v_l(N,K)\equiv\frac{1}{N}\langle\sum_{j=1}^{N}\sigma_j\sigma_{j+l}\rangle, \tag{9}$$

where $K=J/2kT$.

Despite the shift in indices in Eq. (9)

$$\frac{4kT}{(g\beta)^2}\chi(T)=\lim_{N\to\infty}\sum_{l=0}^{N-1}v_l(N,K) \tag{10}$$

since all the pair correlations included in Eq. (8) are correctly included in Eq. (10). In the subsequent treatment, N will be restricted to N even, but this should not affect the result for N infinite. The difference between the solution for N even and N odd goes to zero with increasing N in the case of Ising coupling.[3] Griffiths[10] has shown that in general the free energy of a spin system is proportional to N for large N.

For $2N$ spins arranged in a ring $\sigma_{2N+1}\equiv\sigma_1$. Hence, from the symmetry property $v_l=v_{-l}$, it follows that

$$v_{2N-l}(2N,K)=v_l(2N,K),\quad 0\le l\le N. \tag{11}$$

Hence, from Eq. (10),

$$\frac{4kT\chi(T)}{(g\beta)^2}=\lim_{N\to\infty}[1+2\sum_{l=1}^{N-1}v_l(2N,K)+v_N(2N,K)] \tag{12}$$

$$=\lim_{N\to\infty}\sum_{l=0}^{N-1}[v_l(2N,K)+v_{l+1}(2N,K)]. \tag{13}$$

It should be noted that from Eq. (9) it follows that $v_0(2N,K)=1$. Because the spins are in a ring, all the correlations appear twice except the first and the last. Equation (13) illustrates a property that will be important, namely that the correlations appear in pairs.

We will consider the low-temperature limit of Eq. (13) in order to illustrate what properties of the ordering are important. In this limit it is necessary to first let $N\to\infty$ and then $K\to-\infty$. The conjectures which will be used are

1. $$\lim_{N\to\infty}\sum_{l=0}^{N-1}[v_l(2N,K)+v_{l+1}(2N,K)] =\lim_{N\to\infty}\lim_{N'\to\infty}\sum_{l=0}^{N-1}[v_l(2N',K)+v_{l+1}(2N',K)].$$

[9] R. B. Griffiths, Phys. Rev. **133**, A768 (1964).

[10] R. B. Griffiths, J. Math. Phys. **5**, 1215 (1964).

2. The limit $N\to\infty$ of $v_l(2N,K)$ exists and will be denoted by $v_l(K)$.

3. $|v_{l+1}(K)|<|v_l(K)|$. (14)

4. The correlations alternate in sign; i.e.,

$$v_{2l+1}(K)<0<v_{2l}(K).$$

5. $v_l(K)$ converges uniformly to the zero-temperature correlation ω_l for l contained in all closed intervals of the form $[0,M]$ for any M. This means that for any $\epsilon>0$ there is a K_M depending upon M such that for $|K|>|K_M|$, $|v_l(K)-\omega_l|<\epsilon$ for any $l\leq M$.

6. For any $\epsilon>0$ there is an M_c and K_c such that for $l\geq M_c$ and $|K|\geq|K_c|$, $|v_l(K)+v_{l+1}(K)|<\epsilon$.

7. The second difference of $|v_l(K)|$ because of conjectures 3 and 4 can be written

$$\Delta_2|v_l(K)|\equiv|v_{l-1}(K)+v_l(K)|-|v_l(K)+v_{l+1}(K)|. \quad (15)$$

This second difference as a function of l changes sign a finite number of times.

Because these conjectures will be employed to construct mathematical proofs, they are stated in a form which facilitates their use; however, their content is simple and reasonable. For example, the alternating signs of conjecture 4 are almost certainly necessary if the usual idea of an alternating spin arrangement is in any sense valid. Certainly one expects the correlations to decrease with separation but in Eq. (14) it is further asserted that this decrease is monotonic. Conjecture 6 can be viewed as saying that as the separation becomes very large, the small percentage increase in l caused by increasing it by one causes a very small change in the correlation. In the limit of large l the second difference $\Delta_2|v_l|$ is just the second derivative of $|v_l(K)|$ with respect to l. The pair correlations would have to be very "unsmooth" functions if conjecture 7 is invalid.

The manner in which $v_l(K)$ is presumed to converge to ω_l, conjecture 5, is illustrated in Fig. 1 where $|v_l(K)|$ is compared with $|\omega_l|$. The correlation better and better approximates $|\omega_l|$ for larger and larger l with increasing $|K|$, but for any nonzero temperature it eventually departs from $|\omega_l|$. The rate of this departure is taken to decrease with increasing l and $|K|$; i.e., increasing separation of the pairs and decreasing temperature. In part these conjectures are just a restatement of the idea that the short range order extends to greater distances with decreasing temperature. The rapid broadening for $|K|>1$ of the nuclear resonance line[11] of $CuSO_4\cdot 5H_2O$, a substance approximating a linear chain, in a sense supports conjecture 5, since the linewidth of such a substance is strongly dependent upon the nearer neighbor correlations.

The finite-chain results of Bonner and Fisher[3] support these conjectures. For example, the agreement between the extrapolated finite-N values of ω_l and ω_∞ and their infinite-N value suggests the correctness of the second conjecture. For $N=6$ and $N=10$ the last correlation is larger in absolute value than the next to last. This is probably due to the two possible paths around the chain. Conjecture 3 concerns the infinite N limit, and in the limit this end effect probably vanishes. At $\gamma=1.0$, $(|\omega_5|-|\omega_4)/\omega_4$ for $N=10$ is 30% smaller than $(|\omega_3|-|\omega_2|)/\omega_2$ for $N=6$, and this percentage difference is even greater for smaller values of γ. Fisher[12] has suggested that there is a possibility that conjecture 3 may be incorrect.

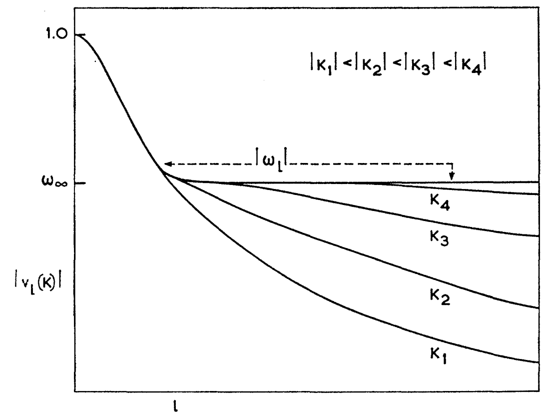

FIG. 1. Approach of $|v_l(K)|$ to $|\omega_l|$ with decreasing temperature; i.e., with increasing $|K|$.

Of the conjectures, the first is probably the least intuitive. By expressing some of the other conjectures in terms of the infinite N limit of $v_l(2N,K)$, conjecture 1 can be eliminated. This has not been done for simplicity and because the different conjectures would only be sufficient and not necessary.

If $v_l(K)$ is continuous, then

$$\lim_{K\to-\infty} v_l(K)=\omega_l. \quad (16)$$

Equation (16) by itself is not sufficient to take the low-temperature limit or, in fact, to provide a satisfactory understanding of the ordering. One question which presents itself is: What is the value of $|v_l(K)|$ in the limit of $l\to\infty$ and then $K\to-\infty$? For Ising coupling,[1]

$$v_l(K)=(-\tanh|K|)^l. \quad (17)$$

Hence,

$$\lim_{K\to-\infty}\lim_{l\to\infty}|v_l(K)|=0 \quad \text{for} \quad \gamma=0. \quad (18)$$

These limits do not give ω_∞ for $\gamma=0$; i.e., unity. The author believes that Eq. (18) is correct for all values of γ. If this is the case, then what is the significance of ω_∞? The above conjectures will provide one answer to this question, give a more complete description of the ordering, and lead to a restriction on the zero-temperature pair correlations.

Note: the following proofs only use conjectures 3 and 4 in their limiting form $K\to-\infty$. They were assumed valid for all K to simplify the proofs slightly and to suggest general properties.

[11] S. Wittekoek, N. J. Poulis, and G. E. Snip, Phys. Letters **11**, 282 (1964).

[12] M. E. Fisher, Phil. Mag. **7**, 1731 (1962).

3. CONSEQUENCES OF THE CONJECTURES

The conjectures are now employed in an investigation of the low temperature limit of Eq. (13). It will be shown that this limit exists even if $\omega_\infty \neq 0$, and bounds on this limit will be found. These bounds are functions of the zero-temperature pair correlations and include ω_∞ in a crucial way.

Using Eq. (13) and the first two conjectures one has

$$4kT\chi(T)/(g\beta)^2 = \sum_{l=0}^{\infty} [v_l(K)+v_{l+1}(K)] \equiv S(K). \quad (19)$$

Because of the pairing property, the general term is $v_l(K)+v_{l+1}(K)$ and not $2v_l(K)$.

In order to show that the sum $S(K)$ converges in the low temperature limit and get bounds on this limit, two preliminary lemmas are necessary.

Lemma 1: For all $\epsilon>0$ there exists an M_1 such that for $M \geq M_1$

$$|V_M(K)-S_M| < \epsilon \quad \text{for} \quad |K| > |K_{M+1}|,$$

where

$$V_M(K) \equiv 1+2\sum_{l=1}^{M} v_l(K)+v_{M+1}(K), \quad (20)$$

$$S_M \equiv 1+2\sum_{l=1}^{M} \omega_l - (-1)^M \omega_\infty. \quad (21)$$

The quantity K_{M+1} depends upon M.

Proof: For convenience the explicit dependence of v_l on K is not shown.

$$|V_M(K)-S_M| = |2\sum_{l=1}^{M}(v_l-\omega_l)+v_{M+1} - \omega_{M+1}+\omega_{M+1}-(-1)^M\omega_\infty| \quad (22)$$

$$\leq 2\sum_{l=1}^{M}|v_l-\omega_l| + |v_{M+1}-\omega_{M+1}| + |\omega_{M+1}-(1)^M\omega_\infty|. \quad (23)$$

By definition there is an M_1 such that for $M \geq M_1$, $|\omega_{M+1}-(-1)^M\omega_\infty| < \epsilon/3$. By conjecture 5 there exists a K_{M+1} depending upon M such that for $|K|>|K_{M+1}|$ and $l \leq M+1$ one has $|v_l-\omega_l| < \epsilon/3(M+1)$. Therefore

$$|V_M(K)-S_M| < \frac{2M+1}{3(M+1)}\epsilon + \frac{\epsilon}{3}$$
$$< \epsilon \text{ for } M \geq M_1, \quad |K| > |K_{M+1}|.$$

Lemma 2: The $\lim_{n\to\infty} S_n$ exists and will be denoted by S_∞, and $S_1 < S_3 < \cdots < S_\infty < \cdots < S_4 < S_2$.

Proof: Equation (21) can be written $S_n = (1-\omega_\infty) + 2\sum_{l=1}^{n} z_l$, where $z_l = \omega_l - (-1)^l \omega_\infty$. Using the asymptotic form of conjectures 3 and 4, one can show that

$$|z_l| = (-1)^l \omega_l - \omega_\infty.$$

Hence $|z_{l+1}|-|z_l| = (-1)^{l+1}(\omega_{l+1}+\omega_l) < 0$ also $z_{2l+1} < 0 < z_{2l}$. Thus S_n is an alternating series of steadily decreasing terms. Therefore,

$$S_1 < S_3 < \cdots < S_{2n+1} < S_{2n} < \cdots < S_4 < S_2. \quad (24)$$

Also $|S_{n+m}-S_n| < 2||\omega_{n+1}|-\omega_\infty|$ for all $m \geq 1$. The convergence now follows from the definition of ω_∞ and the bounds from Eq. (24).

Theorem: $\lim_{K\to-\infty} S(K) = S_\infty$.

Proof: To facilitate the proof, $S(K)$ is divided into 2 parts as follows:

$$|S(K)-S_\infty| = |V_M(K)-S_M+S_M-S_\infty + (v_{M+1}+v_{M+2})+(v_{M+2}+v_{M+3})+\cdots|$$
$$\leq |V_M(K)-S_M| + |S_M-S_\infty| + |\Phi(K)|,$$

where $V_M(K)$ was defined by Eq. (20) and $\Phi(K) = y_{M+1}+y_{M+2}+\cdots$

$$y_l = v_l + v_{l+1}. \quad (25)$$

Note that, as stated in connection with Eq. (19), the general term for large l must be in the form y_l. Because of the decreasing and alternating of v_l the terms y_l also alternate in sign. Further, y_l increases or decreases in magnitude with increasing l in regions in which $\Delta_2|v_l|$ [see Eq. (15)] is negative or positive, respectively. Consider the division of $\Phi(K)$ into partial sums in each of these regions. Because of the monotonic character of y_l in regions in which $\Delta_2|v_l|$ is of constant sign and also because of the alternating signs, the partial sums (and the last infinite sum) are each bounded by the maximum y_l in the region. Hence

$$|\Phi(K)| \leq (p+1)|Q| \leq \epsilon/3,$$

where p is the maximum number of times $\Delta_2|v_l|$ changes sign for any value of K. That such a p exists follows from conjecture 7. The quantity Q is the maximum y_l for $l \geq M$. By conjecture 6 we can choose $M \geq M_c$ and $|K| \geq |K_c|$ so that $(p+1)|Q| < \epsilon/3$.

By Lemma 2, $\quad |S_M - S_\infty| < \epsilon/3$ for $M \geq$ some M_2.

By Lemma 1, $\quad |V_M(K)-S_M| < \epsilon/3$ for $M \geq M_1$ $\quad |K| \geq |K_{M+1}|$.

For

$$M = \max\{M_1, M_2, M_c\}, \quad |K| > \max\{|K_c|, |K_{M+1}|\} \quad (26)$$

all these conditions are simultaneously satisfied. Hence $|S(K)-S_\infty| < \epsilon$ for K satisfying Eq. (26).

Using this theorem, Eq. (19) and the previous definition $K = J/2kT$ one has

$$S_\infty = \lim_{T\to 0} 4kT\chi(T)/(g\beta)^2. \quad (27)$$

Griffiths[9] and Bonner and Fisher[3] have estimated that $J\chi(0)/(g\beta)^2 = 0.05066$ for $\gamma=1$. Bonner and Fisher's work shows that $\chi(0)=0$ for $\gamma<1$. Hence from their work $S_\infty = 0$.

TABLE I. Values of S_n for $n+1$, 2, 3, 4.

γ	S_1	S_2	S_3	S_4	Errors[a]
1.0	-0.184	0.316	-0.068	0.232	± 0.01
0.9	-0.188	0.296	-0.074	0.214	± 0.01
0.8	-0.170	0.260	-0.050	0.176	± 0.01
0.7	-0.137	0.197	-0.021	0.119	± 0.02
0.6	-0.098	0.114	-0.006	0.060	± 0.02
0.5	-0.055	0.039	$+0.001$	0.017	± 0.02
0.4	-0.024	0.008	-0.004	-0.002	± 0.01
0.3	-0.008	0.006	0.000	0.002	± 0.005
0.2	-0.001	-0.001	-0.001	-0.001	± 0.001
0.1	0.000	0.000	0.000	0.000	± 0.0001
0	0	0	0	0	0

[a] Errors in ω_l from Ref. 7. The errors in S_n could be larger.

Note that if one could find the minimum $|K(\epsilon)|$ satisfying Eq. (26), then the theorem provides an upper bound on the susceptibility, namely $2|J|\chi<(g\beta)^2\times\epsilon|K(\epsilon)|$. This could be useful since it is possible that χ vanishes as $K\to\infty$ for Heisenberg coupling.[9,13] From Lemma 2 it follows that

$$S_1<S_3<\cdots<S_\infty=0<\cdots<S_4<S_2. \tag{28}$$

Values of S_n ($n=1$, 2, 3, 4) are shown in Table I based on Bonner and Fisher's values[3,7] of ω_l for various values of γ. The values of S_n bracket zero very closely for $\gamma<0.5$. They violate Eq. (28) by amounts well within the estimated errors[7] in the ω_l's.

Since for $\gamma\neq 1$ the $\lim_{T\to 0}\chi(T)\to 0$ exponentially,[3] it is quite possible that the limiting behavior described by conjectures 5 and 6 is also exponential.

As a demonstration of one use of these relations Table II shows lower bounds on ω_5 based on $|\omega_5|<|\omega_4|$ and upper bounds based on Eq. (28); i.e.

$$S_5=S_4+2(\omega_5+\omega_\infty)<0, \tag{29}$$

$$\omega_5<-\tfrac{1}{2}S_4-\omega_\infty. \tag{30}$$

For comparison purposes values of $-\omega_\infty$ are also shown as upper bounds. It is seen that Eq. (30) gives much better bounds.

TABLE II. Bounds on ω_5.

γ	Lower bound $-\omega_4$	Upper bound $-S_4/2-\omega_\infty$	Upper bound $-\omega_\infty$	Errors[a]
1.0	-0.150	-0.116	-0.000	± 0.01
0.9	-0.180	-0.143	-0.036	± 0.01
0.8	-0.225	-0.198	-0.112	± 0.01
0.7	-0.297	-0.287	-0.227	± 0.02
0.6	-0.405	-0.402	-0.372	± 0.02
0.5	-0.545	-0.546	-0.537	± 0.02
0.4	-0.695	-0.693	-0.694	± 0.01
0.3	-0.825	-0.825	-0.824	± 0.005
0.2	-0.921	-0.920	-0.921	± 0.001
0.1	-0.980	-0.980	-0.980	± 0.0001
0	-1.0	-1.0	-1.0	0

[a] Errors in ω_l from Ref. 7. The errors in the bounds could be larger.

[13] Z. G. Soos, J. Chem. Phys. 43, 1121 (1965).

Because of conjecture 3, the absolute value of the correlation $|v_l|$ is a decreasing function of l. If the further conjecture is made that the rate of this decrease is monotonic, then $\Delta_2|v_l|>0$. With this added condition a simple proof shows that Eq. (28) is also correct if S_n is replaced by

$$G_n=\sum_{l=0}^{n}(\omega_l+\omega_{l+1}). \tag{31}$$

Conjecture 6 is necessary to prove the convergence of G_n, but is not necessary to obtain the bounds.

Because this conjecture, $\Delta_2|v_l|>0$, can be seen from Eq. (17) to be correct for Ising coupling one might think it is generally correct. However, using Bonner and Fisher's values one finds that $G_3>0$ for γ greater than about 0.5; i.e., the inequality is not satisfied. Hence, for these values of γ, it is likely that the slope of $|v_l|$ is not monotonic. This implies that $\Delta_2|v_l|$ has at least two zeros near the Heisenberg limit. These zeros probably occur at relatively small l values before v_l takes on an asymptotic form.[12] Conjecture 7 depends upon the large l behavior.

4. DISCUSSION

A reasonable set of conjectures concerning the pair correlations which provides a general picture of the ordering has led to a set of inequalities, Eq. (28). These conjectures are merely sufficient to derive Eq. (28). Slightly different conjectures would also lead to this equation. It is hoped that future work will verify these conjectures and that Eq. (28) can be used as a rigorous relation to test approximate calculations. Equation (28) can also be used to place upper bounds on ω_∞ if accurate values of ω_l become available.

The inequalities are consistent with present predictions for the quantities involved. This agreement suggests the validity of the conjectures made. In the inequalities and their derivation, ω_∞ plays a fundamental role. This role partially explains the importance of ω_∞ even though $\lim_{l\to\infty}|v_l(K)|$ is probably zero for $T\neq 0$.

When the correlations approximate their zero-temperature values out to a distance ξ such that $|\omega_\xi|\approx\omega_\infty$ and decrease slowly thereafter with increasing separation, then $T\chi$ is approximately zero. This follows from the proof of the theorem. In the worst case, $\gamma=1.0$, ω_4 is already within 15% of $\omega_\infty=0$. Therefore, it seems reasonable that values as small as 20 may suffice for ξ. The correlations v_l for $l>\xi$, which are, in general, less than ω_∞, tend to cancel one another in pairs.

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