Helical order and its onset at the Lifshitz point*

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We study the helical phase and the Lifshitz point for a model system with competing ferromagnetic and antiferromagnetic interactions by using high-temperature series techniques. We locate the Lifshitz point, and we find the exponent that characterizes the vanishing of the wave vector $\vec{q}_0$ associated with the helical phase as the Lifshitz point is approached. In the helical phase we determine the dependence of $\vec{q}_0$ on the competing interactions, and we estimate the structure factor exponent.

Recently, the phenomena associated with helical order have been the focus of renewed investigation. Helical order was first discovered independently by Kaplan,[1] Villain,[2] and Yoshimori[3] who used mean-field theory to study magnetic systems in which the mechanism for helical order is competition between ferromagnetic and antiferromagnetic interactions. It was found that for a certain range of values of the exchange interactions, a helical phase is energetically favored over a ferromagnetic phase. The helical phase is characterized by a magnetization that varies sinusoidally in space with an associated wave vector $\vec{q}_0$ that is a continuous function of the exchange interactions.[4-7]

The point in the phase diagram where $\vec{q}_0 \rightarrow 0$, is particularly interesting. The importance of this point, the Lifshitz point, was first stressed by Hornreich *et al.*[8] because a new type of critical behavior occurs at this coexistence between disordered, ferromagnetic, and helical phases. Very recently, there have been several theoretical investigations which indicate that Lifshitz points can be attained in liquid crystals,[9-11] and this appears to be confirmed experimentally.[12]

In this article we report the results of the first high-temperature series investigation of a model system which exhibits a Lifshitz point and a helical phase. Our studies are the first to show quantitatively the non-mean-field character of the Lifshitz point, and the variation of $\vec{q}_0$ in the helical phase. We also calculate T_c accurately and show that, contrary to widespread belief, T_c does not achieve a minimum at the Lifshitz point.

We study the model system with the following n-vector Hamiltonian[13]:

$$\mathcal{H} = -J_{xy}\sum_{\langle ij\rangle}^{xy} \vec{S}_i\cdot\vec{S}_j - J_z\sum_{\langle ij\rangle}^{z} \vec{S}_i\cdot\vec{S}_j - J_z'\sum_{[ij]}^{2z} \vec{S}_i\cdot\vec{S}_j, \quad (1)$$

where the first two sums are over nearest-neighbor spin pairs in the same x-y plane and in adjacent x-y planes, respectively, and the third sum is over next-nearest-neighbor pairs along the z axis.

The type of ordered phases that occurs in this model depends on the values of $R \equiv J_z/J_{xy}$ and $S \equiv J_z'/J_{xy}$; for sufficiently negative $S/|R|$, a helical phase is energetically favored. In mean-field theory the helical phase occurs for $S < -\frac{1}{4}|R|$ [cf. Fig. 1(a)], and the wave vector q_0 (which is along the z axis) associated with the helical magnetization $\tilde{M}$ is $\cos^{-1}(-|R|/4S)$. Near the critical point, fluctuations of wave vector q_0 become large, and as $T \rightarrow T_c$, the response of $\tilde{M}$ with respect to its conjugate field $\tilde{H}$ diverges in a manner analogous to the divergence of $\partial M/\partial H$ for a ferromagnetic system. Thus a study of $\partial\tilde{M}/\partial\tilde{H}$ is necessary in order to understand the phase transition in the helical phase. It will prove useful to write $\partial\tilde{M}/\partial\tilde{H}$ in terms of the structure factor $\mathcal{S}(\vec{q}_0)$,

$$\frac{\partial\tilde{M}}{\partial\tilde{H}} \equiv \mathcal{S}(\vec{q}_0) = \sum_{\vec{r}} \langle s_0 s_{\vec{r}}\rangle e^{i\vec{q}_0\cdot\vec{r}} = \sum_{\vec{r}} \langle s_0 s_{\vec{r}}\rangle e^{iq_0 z}. \quad (2)$$

In this form we can investigate the Lifshitz point, where $q_0 \rightarrow 0$, by expanding $\mathcal{S}(q)$ for small q:

$$\mathcal{S}(q) = \sum_{\vec{r}} \langle s_0 s_{\vec{r}}\rangle \left(1 \frac{-q^2 z^2}{2} + \frac{q^4 z^4}{4!}\cdots\right) \quad (3a)$$

$$\equiv \chi - \tfrac{1}{2}q^2\langle z^2\rangle + \frac{q^4\langle z^4\rangle}{4!}\cdots . \quad (3b)$$

The second equality defines the z moments of $\langle s_0 s_r\rangle$, and $\chi = \mathcal{S}(0)$ is the reduced susceptibility. Taking the inverse of (3), we write $\mathcal{S}(q)^{-1}$ as a Landau-like expansion with q playing the role of an order parameter,

$$\mathcal{S}(q)^{-1} = \chi^{-1}\left[1 + \frac{q^2\langle z^2\rangle}{2\chi} + q^4\left(\frac{\langle z^2\rangle^2}{4\chi^2} - \frac{\langle z^4\rangle}{24\chi}\right) + \cdots\right]. \quad (4)$$

When ferromagnetic order occurs, $\mathcal{S}(q)^{-1}$ has a minimum at $q_0 = 0$, and at T_c, $\chi^{-1} = 0$. However, if the coefficient of q^2 in (4) is negative, then $\mathcal{S}(q)^{-1}$ is a minimum at nonzero q_0 and helical order re-

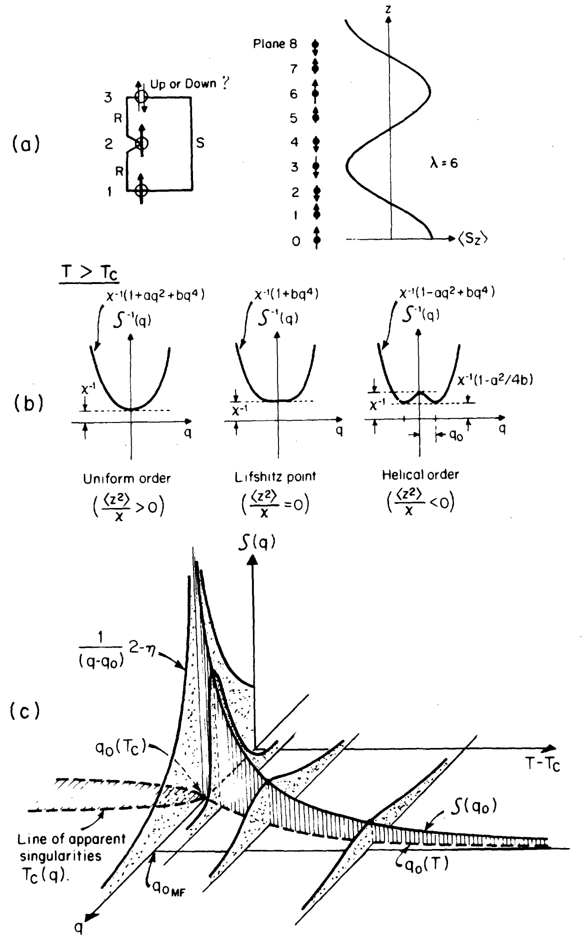

FIG. 1. A summary of the qualitative features of the model system: (a) The competing nature of the interactions for $R > 0$, $S < 0$. If spins 1 and 2 are pointing up, then the effect of the R interaction is to point spin 3 up, while the S interaction has the opposite effect. To the right, a typical example of a helical phase is shown for Ising spins. Each dot represents one x-y plane, and the length of the arrow is proportional to the spin expectation value $\langle s_z \rangle$ in each x-y plane. (b) The dependence of the inverse structure factor on q for fixed $T > T_c$. Note the analogy with Landau theory. (c) A schematic plot of the structure factor $S(q,T)$. At high temperature, the peak of $S(q)$ occurs at $q_0^{\mathrm{MF}} = \cos^{-1}(-|R|/4S)$, and as T decreases this peak moves to lower q for $S \gtrsim -0.65$, and to higher q for $S \lesssim -0.65$. Extrapolating series for $S(q)$ gives rise to a line of apparent singularities in the T-q plane, and the peak of this curve locates q_0 at T_c.

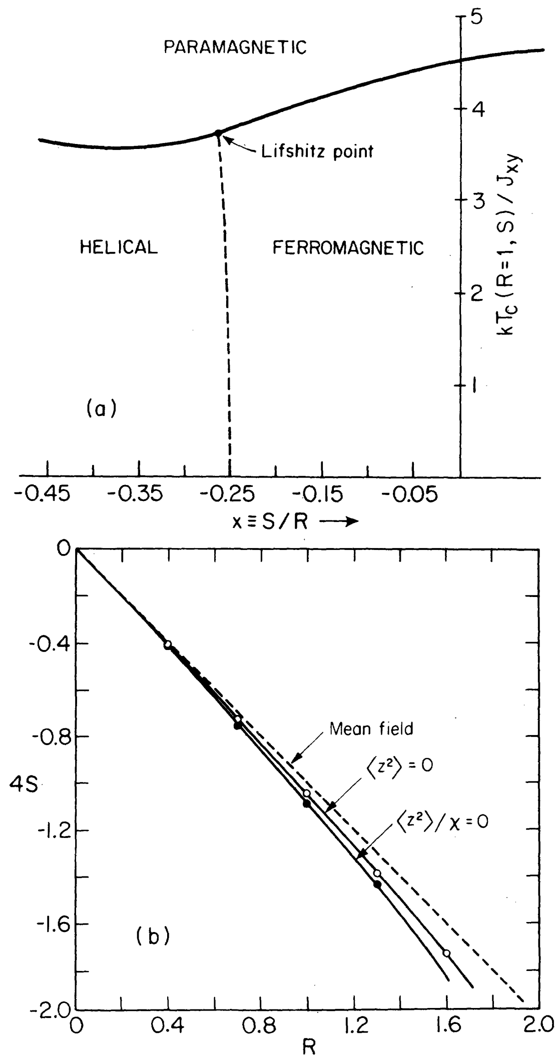

FIG. 2. (a) Schematic phase diagram for the system modeled by the Hamiltonian (1). The dashed line represents a first-order transition, while our $n = 1$ data for the second-order line are shown as a solid line. As R varies, the Lifshitz point becomes a "Lifshitz boundary." (b) Estimates for the Lifshitz boundary based on the two equivalent criteria $\langle z^2 \rangle / \chi = 0$ and on $\langle z^2 \rangle = 0$. The Lifshitz boundary predicted by mean-field theory is shown for comparison.

sults [cf. Fig. 1(b)]. The vanishing of the coefficient of q^2 in (4) is therefore the transition between helical and ferromagnetic order. Thus we may locate a line of Lifshitz points in R-S space, the "Lifshitz boundary," by the condition $\langle z^2 \rangle / \chi = 0$ or, equivalently, $\langle z^2 \rangle = 0$. Furthermore, by minimizing $S(q)^{-1}$ with respect to q^2, we find asymptotically

$$q_0^2 \sim 6\langle z^2 \rangle \chi / (\langle z^4 \rangle \chi - 6\langle z^2 \rangle^2). \tag{5}$$

To study the properties associated with the Lifshitz point, we have used linked cluster theory[14] to calculate high-temperature series for χ, $\langle z^2 \rangle$, and $\langle z^4 \rangle$ to order 8 in powers of $\beta \equiv 1/kT$ for Ising spins ($n = 1$). The series for $\langle z^2 \rangle$ and $\langle z^4 \rangle$ are given in Tables I and II, respectively.[15] The result of our analysis for the location of the Lifshitz boundary is shown in Fig. 2. Figure 3 shows that as the Lifshitz point is approached, $q_0 \sim A(x - x_L)^{\beta_q}$ with an exponent β_q of 0.5 ± 0.15; here $x \equiv S/R$ and x_L de-

TABLE I. The coefficients C_{jkl} in the reduced-second-moment series.

$$\langle z^2 \rangle = \sum_{l=0}^{\infty} \sum_{j+k \le l} C_{jkl} \tanh^{l-j-k}(\beta J_{xy}) \tanh^{j}(\beta J_z) \tanh^{k}(\beta J_z').$$

$l \backslash j$	0	1	2	3	4	5	6	7	8
				$k=0$					
0	0								
1	0	2							
2	0	16	8						
3	0	80	96	18					
4	0	336	672	304	32				
5	0	1 264	3 680	2 816	704	50			
6	0	4 432	17 376	19 504	8 256	1 360	72		
7	0	14 768	74 208	112 432	70 208	19 424	2 336	98	
8	0	47 376	294 624	572 464	484 864	197 584	39 456	3 696	128
				$k=1$					
1	8								
2	64	40							
3	320	480	112						
4	1 344	3 360	1 920	232					
5	5 056	18 400	17 792	5 376	400				
6	17 728	86 880	123 008	63 744	11 904	616			
7	59 072	371 040	707 840	542 912	175 680	22 528	880		
8	189 504	1 473 120	3 597 952	3 471 728	1 807 232	402 304	38 272	1192	
				$k=2$					
2	32								
3	384	208							
4	2 688	3 360	640						
5	14 720	30 368	14 336	1 360					
6	69 504	206 432	165 696	41 312	2 368				
7	296 832	1 176 320	1 385 472	604 096	92 928	3 664			
8	1 178 496	5 936 608	9 418 112	6 141 280	1 687 808	177 408	5 248		
				$k=3$					
3	72								
4	1 216	632							
5	11 264	13 280	2 320						
6	78 016	150 240	65 152	5 304					
7	449 728	1 240 160	913 920	202 008	9 408				
8	2 289 856	8 379 040	9 057 664	3 569 408	475 008	14 648			
				$k=4$					
4	128								
5	2 816	1 440							
6	33 024	37 920	6 352						
7	280 832	523 328	217 088	16 032					
8	1 939 456	5 148 064	3 620 672	747 104	29 120				
				$k=5$					
5	200								
6	5 440	2 760							
7	77 696	88 032	14 416						
8	790 336	1 446 688	585 088	40 584					
				$k=6$					
6	288								
7	9 344	4 720							
8	157 824	177 440	28 672						
				$k=7$					
7	392								
8	14 784	7 448							
				$k=8$					
8	512								

TABLE II. The coefficients D_{jkl} in the reduced-fourth-moment series.

$$\langle z^4 \rangle = \sum_{l=0}^{\infty} \sum_{j+k\leq l} D_{jkl} \tanh^{l-j-k}(\beta J_{xy}) \tanh^{j}(\beta J_z) \tanh^{k}(\beta J_z').$$

$l \backslash j$	0	1	2	3	4	5	6	7	8
				$k=0$					
0	0								
1	0	2							
2	0	16	32						
3	0	80	384	162					
4	0	336	2 688	2 608	512				
5	0	1 264	14 720	23 552	10 496	1 250			
6	0	4 432	69 504	160 048	117 504	31 312	2 592		
7	0	14 768	296 832	911 920	964 352	421 472	76 928	4 802	
8	0	47 376	1 178 496	4 602 160	6 493 696	4 085 968	1 214 592	164 976	8 192
				$k=1$					
1	32								
2	256	328							
3	1 280	3 936	1 600						
4	5 376	27 552	26 112	5 320					
5	20 224	150 880	237 056	111 744	13 888				
6	70 912	712 416	1 616 384	1 263 744	360 960	30 664			
7	236 288	3 042 528	9 227 264	10 428 992	4 942 080	956 800	59 968		
8	758 016	12 078 584	46 628 376	70 446 752	48 338 432	15 504 640	2 192 396	107 080	
				$k=2$					
2	512								
3	6 144	4 240							
4	43 008	67 872	18 688						
5	235 520	610 976	389 120	58 768					
6	1 112 064	4 141 664	4 367 616	1 541 216	148 480				
7	4 749 312	23 561 984	35 825 664	21 084 352	4 758 528	321 424			
8	18 855 936	118 768 096	240 857 600	205 580 896	77 806 592	12 269 568	620 800		
				$k=3$					
3	2 592								
4	41 728	24 536							
5	376 832	495 968	115 648						
6	2 560 768	5 489 760	2 951 680	375 384					
7	14 590 720	44 618 720	39 684 096	11 926 144	963 840				
8	73 634 560	298 241 824	382 199 296	192 732 032	37 246 464	2 106 200			
				$k=4$					
4	8 192								
5	167 936	92 448							
6	1 880 064	2 286 624	489 280						
7	15 429 632	30 337 088	14 913 536	1 700 640					
8	103 899 136	289 959 328	235 291 904	63 933 536	4 537 088				
				$k=5$					
5	20 000								
6	500 992	266 856							
7	6 743 552	7 869 792	1 603 264						
8	65 375 488	122 642 848	57 193 984	6 076 176					
				$k=6$					
6	41 472								
7	1 230 848	643 504							
8	19 433 472	22 139 168	4 376 320						
				$k=7$					
7	73 832								
8	2 639 616	1 364 216							
				$k=8$					
8	131 072								

notes the Lifshitz point. Our result is consistent with renormalization-group calculations[8] which predict $\beta_q = 0.5 + O(\epsilon^2)$, where $\epsilon = 4 - d$.

To study the helical phase, where q_0 is not necessarily small, we calculated and analyzed series for the full structure factor *for arbitrary q* for Ising spins to order 8. We investigated the dependence of q_0 on R, S, and temperature, by studying the coefficients $a_l(q)$ in the series for $\mathcal{S}(q) = \sum_{l=0}^{L} a_l(q)\beta^l$. In particular, the series coefficient $a_1(q) = J_{xy}(4 + 2R\cos q + 2S\cos 2q)$ is identical to $a_1(q)$ in mean-field theory, and therefore $a_1(q)$ versus q has a maximum at $q_0 = \cos^{-1}(-|R|/4S)$. For the representative case $R = 1$, we find that for $S \gtrsim -0.65$, the peak of $a_l(q)$ vs q occurs at progressively lower q as l increases, while when $S \lesssim -0.65$, the peak of $a_l(q)$ vs q moves to higher q. Thus we find that the peak of $\mathcal{S}(q)$ vs q is in general temperature dependent [cf. Fig. 1(c)].

Our estimate for q_0 at T_c is based on observing [cf. Eq. (4)] that $\mathcal{S}(q_0)$ diverges at T_c, while for $q \neq q_0$, $\mathcal{S}(q)$ extrapolates to an apparent divergence at a lower temperature. Therefore q_0 can be found by locating the peak of $T_c(q)$ vs q. Furthermore, the Lifshitz point may be found, independent of our previous method, by varying R and S so that the peak of $T_c(q)$ vs q tends to zero. From this method we find the Lifshitz point occurs at $S = -0.271 \pm 0.002$ for $n = 1$, and Fig. 3 shows q_0^2 vs $x \equiv S/R$.

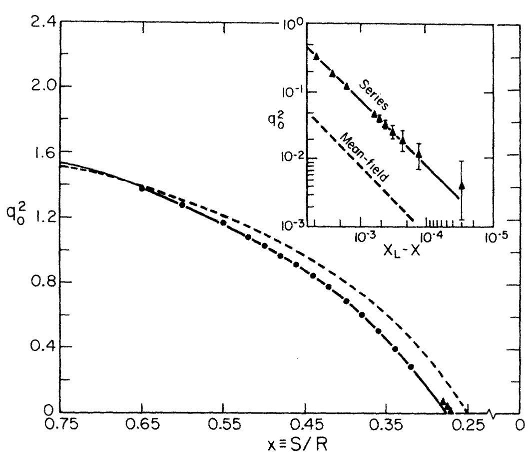

FIG. 3. Helical phase wave vector squared vs $x \equiv S/R$ for the case of Ising spins and $R = 1$. Shown are the mean-field prediction $q_0 = \cos^{-1}(-|R|/4S)$ (dashed), the prediction based on the location of the peak of $T_c(q)$ vs q (solid), and the prediction based on minimizing the small-q expansion of Eq. (4) (triangles). The inset shows the data in more detail near the Lifshitz point. The data lie on a straight line of slope unity, indicating that $q_0 \sim A(x - x_L)^{1/2}$.

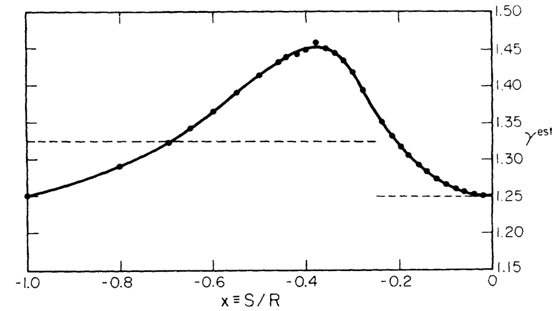

FIG. 4. Estimated exponent γ^{est} of $\mathcal{S}(q)$ for the case of Ising spins and $R = 1$. The dashed line is the renormalization-group prediction (Refs. 6 and 7).

Finally, we show the results of our analysis for the structure factor exponent γ in Fig. 4. Note the apparently continuous dependence of γ on S. The interpretation of our data requires care in light of renormalization-group predictions that the exponent changes discontinuously at the Lifshitz point. The origin of the apparently continuous variation stems from the fact that competition between the interactions R and S sharply reduces the correlation length in the z direction. This means that near the Lifshitz point, criticality is not evident until one probes closer to T_c than one must probe for the case $S = 0$, and hence longer series are required to probe the asymptotic behavior. This effect is in fact observed upon calculating and analyzing very lengthy series (35 terms) based on an exact solution of (1) in the spherical model limit ($n \to \infty$).[15] This analysis demonstrates that in the ferromagnetic phase, the apparent continuous variation of γ with x is spurious. Thereby we estimate the $n = 1$ structure factor exponent to be 1.25 ± 0.5 for $|x| < |x_L|$, and 1.35 ± 0.05 for $|x| > |x_L|$. These estimates are consistent with renormalization-group predictions[6,7] that for n-component spins the structure factor exponent for $|x| > |x_L|$ is equal to the susceptibility exponent for $2n$-component spins.

For completeness, we have also studied the Hamiltonian (1) for planar and Heisenberg spins ($n = 2, 3$) to orders 6 and 5, respectively. The results obtained were qualitatively similar to the Ising case, and therefore the extensive labor required for longer series was not necessary. In particular, our estimates for the location of the Lifshitz point for $R = 1$ are $S = -0.263 \pm 0.002$ and $S = -0.259 \pm 0.002$ for $n = 2$ and 3, respectively. For the $n = 3$ system, we find no evidence for the predicted[6,7] first-order phase transition from the paramagnetic to helical phases [cf. Fig. 2(a)].

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