DEPENDENCE OF CRITICAL INDICES ON A PARAMETER*

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A number of lattice models of phase transitions and critical points can be related to one another by variation of linear parameters appearing in the Hamiltonian. It is suggested that the critical indices as functions of these parameters remain constant except possibly at points where the nature of the associated first-order phase transition is itself altered by varying a parameter. Several models exhibiting critical phenomena are consistent with this proposal.

At present it is fashionable to analyze critical phenomena in terms of certain indices α, β, γ, δ, ν, etc. which describe the rate of divergence of certain thermodynamic derivatives or ranges of correlation functions upon approaching a critical point.[1] Theoretical estimates for these indices, coming largely from analyses of various lattice systems (Ising, Heisenberg, etc.) suggest that they are largely independent of the details of the system Hamiltonian. The indices do, however, depend on (a) the lattice dimensionality d, (b) the "symmetry of the order parameter" in the sense that, for example, Heisenberg and Ising model indices are unequal, and (c) the range of interaction, provided it decreases sufficiently slowly with distance. To these might be added a fourth effect: the "renormalization" of critical indices by imposition of a constraint involving one or more extensive thermodynamic variables.[2] As renormalization can be understood in terms of straightforward thermodynamic arguments, we shall not consider it further; all our comments below refer to the "unrenormalized" exponents.

We shall show that changes (a), (b), and (c) above can be regarded as arising when a certain linear parameter in the system Hamiltonian achieves a particular value, and that changes in the character of the basic first-order phase transition "underlying" the critical point usually take place at the same parameter value. Our approach is phenomenological and we are unable to predict values for the changes of critical indices. Nonetheless, this viewpoint may suggest a deeper connection between the three (known) causes of critical index change than has heretofore been suspected. It also provides a basis for making an educated guess about the alteration or identity of critical indices in cases where numerical studies have not been carried out or yield uncertain results.

(A) As an example of our procedure, consider an Ising model on a simple-cubic lattice with nearest-neighbor ferromagnetic exchange, but with the exchange interaction J between spins lying in the same layer differing from the exchange J' between spins in adjacent layers, Fig. 1(a). With J constant, let J' decrease to zero; the Curie temperature will presumably decrease continuously to the positive value associated with a simple layer structure, Fig. 1(b). In this figure a magnetic field axis has been added and the cross-hatched region at $H=0$ lying beneath the line of critical points for $J'>0$ is a "coexistence" surface in that the two "phases" of spin up and spin down in the spontaneously magnetized state coexist along this surface. According to current ideas on the subject, the critical indices should retain their three-dimensional values for all $J'>0$ and only revert to the (quite different) two-dimensional values precisely at $J'=0$. What we wish to point out is that if we consider $J'<0$, the whole nature of the phase transition in the HT plane (at constant J') is altered. This arises from the fact that with $J'<0$ the predominant spin direction in the ordered state with $H=0$ alternates up-down-up-down in consecutive layers, while the magnetic field tends to force spins in all the layers to point up (or down, depending on the sign of H). While the detailed phase diagram is not known, it probably resembles that of certain metamagnetic materials.[3] In Fig. 1(b) the dotted lines indicate portions of the phase boundary at $T=0$ and $H=0$ which are known exactly: the $T=0$ lines determined by energy considerations, and

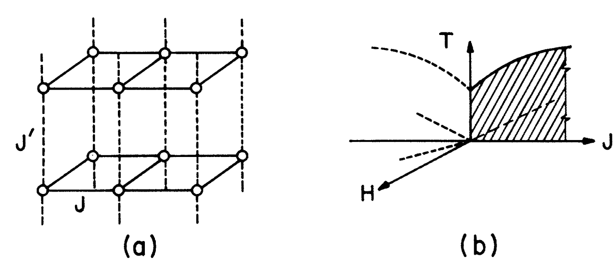

FIG. 1. Phase diagram for cubic Ising ferromagnet with fixed intralayer and variable interlayer exchange.

the $H=0$ line which is simply the mirror image of the critical line for $J'>0$.

This suggests what may be a fairly general rule: Critical indices along a line of critical points terminating a first-order phase-transition surface remain unaltered[4] unless the basic character of the phase transition itself is altered, as is clearly the case at $J'=0$ in the model just considered. Note that the critical indices need not be different at the point where a change occurs; consider, for example, a case like that in the preceding paragraph, but with only two layers (rather than an infinite number), for which both $J'=0$ and $J'>0$ would (according to current ideas) have two-dimensional critical indices, whereas the phase diagram should not differ radically from that shown in Fig. 1(b) (one might expect $dT_c/dJ'=0$ at $J'=0$).

(B) Consider next the dependence of critical indices on the "symmetry of the order parameter" in the Hamiltonian

$$\mathcal{H}=-J\sum_{\langle ij\rangle}\{S_{ix}S_{jx}+S_{iy}S_{jy}+(1+J')S_{iz}S_{jz}\}-H\sum_i S_{iz}, \qquad (1)$$

with the sum over nearest-neighbor sites on a lattice of dimension $d\geqslant 3$. Jasnow and Wortis[5] have argued that at least in the case where $\vec{S}_i$ are classical unit vectors (moving on the surface of a sphere), the critical indices change from Ising-like at $J'>0$ to Heisenberg-like at $J'=0$, and this conclusion seems consistent with the results of Obokata, Ono, and Oguchi,[6] who analyzed (1) in the spin-$\frac{1}{2}$ case. The phase diagram should resemble Fig. 1(b) because for small negative J' the spontaneous magnetization will tend to lie in the xy plane rather than parallel to the z direction, so that the field H is no longer the thermodynamic conjugate to the order parameter. Other cases considered by Jasnow and Wortis may be discussed in a similar fashion.

(C) The Ising linear chain with ferromagnetic interactions decreasing as $r^{-1-\epsilon}$, with r the distance between spins, is known to have a first-order phase transition[7] for $0<\epsilon<1$. The numerical studies by Nagle and Bonner[8] indicate critical indices varying continuously with ϵ in the range $0\lesssim\epsilon<1$. Note that ϵ is not a parameter which appears linearly in the Hamiltonian. For our purposes it is convenient to consider a linear chain with Hamiltonian

$$\mathcal{H}=\sum_{i\neq j}\{J/r_{ij}^{1+\epsilon}+J'/r_{ij}^{1+\epsilon'}\}\sigma_i\sigma_j, \qquad (2)$$

where $\sigma_i=\pm1$ are the Ising spin variables, and $J>0$. For $J'>0$, the ground state of the chain is ferromagnetic (all spins parrallel) and the same is true when J' is slightly negative provided $\epsilon'>\epsilon$ or $\epsilon'>1$. However for $\epsilon'<\epsilon$ and $0<\epsilon'\leqslant 1$, even a small negative J' leads to a ground state consisting of up spins and down spins in alternating blocks, the length of a block increasing as $|J'|/J\to 0$. This strongly suggests (though it does not prove) that the phase diagram is analogous to Fig. 1(b) in that the nature of the first-order phase transition changes character at $J'=0$ for $0<\epsilon<1$, which is consistent with our proposal and the observed variation of indices with ϵ if one makes the reasonable assumption that for $J'>0$ the critical indices are appropriate to the force of longer range (i.e., correspond to ϵ' rather than ϵ).

(D) Ising ferromagnets with next-nearest-neighbor interactions, and, indeed, any set of ferromagnetic pair interactions of finite range, should have the same critical indices as found for the nearest-neighbor case. This result, based on numerical studies,[9] is consistent with our postulate. Thus if J' is the strength of the next-nearest-neighbor interaction on, say, a square or cubic lattice, making it slightly negative should not change the ferromagnetic nature of the phase transition (it certainly does not alter the ferromagnetic ground state). Hence both coexistence surface and critical line should pass smoothly through $J'=0$. The Lee-Yang theorem[10] shows that the transition remains ferromagnetic for all $J'>0$; thus the result stated in the first sentence of this paragraph is very plausible within the framework of our phenomenological considerations.

(E) Ising ferromagnets with spin $S>\frac{1}{2}$; i.e., $S=1$, $\frac{3}{2}$, 2, etc., but with $S<\infty$, should have the same indices as $S=\frac{1}{2}$ on the same lattice.[11] Note that an Ising spin $S>\frac{1}{2}$ can be obtained by coupling clusters of $S=\frac{1}{2}$ spins with ferromagnetic bonds,[12] and using the results of (D) above.

(F) The infinite-spin Ising ferromagnet obtained by replacing $\sigma_i=\pm1$ by a continuous variable $-1\leqslant x_i\leqslant 1$, is not covered by (E). Consider, however, the infinite-spin Hamiltonian

$$\mathcal{H}=-J\sum_{\langle ij\rangle}x_i x_j-D\sum_i x_i^2 \qquad (3)$$

which goes over into the $S=\frac{1}{2}$ case as $D\to\infty$. Letting a parameter approach infinity involves some subtleties, and there are cases where critical indices are believed to change in such a limit.[13]

However, these are situations where letting the parameter go to infinity serves to produce very long-range effects in which behavior of one portion of the lattice may be strictly constrained by choosing appropriate conditions at distant boundaries. Such is not the case with (3), where letting $D\to\infty$ produces a local rather than long-range constraint. Hence we expect the indices for Ising $S=\infty$ to be the same as $S=\frac{1}{2}$, and recent calculations[14] have tended to remove the small discrepancy suggested in Ref. 5. It may be added that the continuity of critical indices when a parameter becomes infinite in the sense of D in (3) is supported by numerical work[15] showing the (apparent) identity of indices for the "xy" model and the "planar" model, the latter being obtained from the former (we here consider the S_i as classical unit vectors) by letting $D\to\infty$ in

$$\mathcal{H}=-J\sum_{\langle ij\rangle}(S_{ix}S_{jx}+S_{iy}S_{jy})+D\sum_i(S_{iz})^2.$$

(G) A Heisenberg model with spin $S>\frac{1}{2}$ can be obtained by coupling together clusters of $S=\frac{1}{2}$ spins with ferromagnetic Heisenberg interactions which must, however (in contrast to the Ising case), be allowed to become infinite. The situation is analogous to that discussed in (F) above, and thus we think it plausible that if the $S=\frac{1}{2}$ Heisenberg model with ferromagnetic interactions of finite range has the same indices as the model with nearest-neighbor interactions alone [itself a reasonable conjecture from our postulates, following the reasoning in (D) above], all Heisenberg ferromagnets with finite spin and finite range of interaction should have the same critical indices. Numerical investigations at present support exceptional behavior for the nearest-neighbor $S=\frac{1}{2}$ case,[16] but due to the difficulty in analyzing these series we do not believe a contradiction with our ideas has been definitively established.

(H) For Ising ferromagnets with long-range interaction decreasing as $r^{-d-\epsilon}$ on lattices of dimension $d\geqslant 2$, considerations similar to those in (C) above suggest that for $\epsilon>1$ the critical indices will be the same as those which arise with only nearest-neighbor interactions present. This prediction differs from the results obtained by Joyce[17] for the spherical model: γ varying with ϵ in the range $1<\epsilon<2$ for $d=2$ and $1.5<\epsilon<2$ for $d=3$ (for smaller values of ϵ, $\gamma=1$). The difference can be traced to the fact that the Ising ferromagnetic ground state is more stable than that of the spherical model against weak long-range antiferromagnetic interactions. The Heisenberg model should resemble the spherical rather than the Ising model in this respect. It is tempting to conjecture that the Ising indices switch abruptly from nearest-neighbor values with $\epsilon>1$ to classical values for $\epsilon<1$, with possibly special values at $\epsilon=1$.[18] Our approach suggests that changes in Heisenberg-model indices could also occur for $1<\epsilon<2$ as well as $0<\epsilon\leqslant 1$.

(I) Although they are not lattice systems, we remark that the failure to observe a "quantum effect" in critical indices for monatomic gases[19] (the parameters of interest are the coefficients of terms in the interatomic potential, together with the inverse mass) lends support to our proposal that critical indices remain the same if there is no fundamental change in the underlying phase transition. In addition, there are a number of systems (binary liquid mixtures and antiferromagnets in an external field) where the critical point seems to be smoothly dependent on parameters which can readily be changed in the laboratory. Although we know of no systematic investigation of critical indices as functions of these parameters, we also know of no instances where they have been observed to change, at least away from regions where the nature of the first-order phase transition is itself changing.

A suitable conclusion to this paper would be a suggestion as to why a term which, when added (in a small amount) to the Hamiltonian with one sign alters the nature of the phase transition, will change the critical indices when added with the opposite sign. Unfortunately, we have no good ideas in this connection and would welcome suggestions by those who have achieved some deeper understanding of the subject.

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EVIDENCE FOR LARGE SPIN-ORBIT COUPLING IN METALLIC MOLYBDENUM*

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We report accurate measurements of the caliper dimensions of the molybdenum Fermi surface. From these measurements, we estimate the separation between the electron jack and the hole octahedra along the $\langle 100\rangle$ directions to be $(7.5\pm1)\%$ of the ΓH dimension. This large separation implies that spin-orbit coupling is much greater than expected for metallic molybdenum.

Considerable effort has been directed toward obtaining an understanding of the itinerant rather than localized character of the d electrons of the chromium-group metals: chromium, molybdenum, and tungsten. These three metals are particularly interesting because of the reported similarity of their paramagnetic energy-band structures and Fermi surfaces.[1] One aspect of the electronic structure concerns the significance and magnitude of spin-orbit coupling effects on the d-like conduction electrons. For the chromium-group metals, this information can be obtained from an accurate determination of the larger Fermi-surface pieces. Figure 1 is a $\langle 110\rangle$ section for the major Fermi-surface pieces for these metals, as proposed by Lomer[2] and verified by Loucks.[1] These major pieces consist of an electron surface in the shape of a child's toy jack at the center (Γ) of the Brillouin zone and octahedrally shaped hole surfaces centered at points H. In the absence of spin-orbit coupling, the jack and octahedra contact along ΓH directions. If spin-orbit coupling exists, however, the jack and octahedra are separated by a gap. This gap is attributed to spin-orbit splitting of the degenerate Δ_5 energy band at the Fermi energy. From a knowledge of this gap dimension and of the detailed energy-band structure along Δ (along ΓH), it is possible to estimate the magnitude of the spin-orbit splitting.

Since tungsten is the heaviest of the chromium-group metals, it would be expected to exhibit the largest spin-orbit coupling effects. That is, one would expect the separation between the jack and the octahedra to be the greatest for tungsten since the spin-orbit splitting of the Δ_5 state should be the largest. On the basis of a radio-

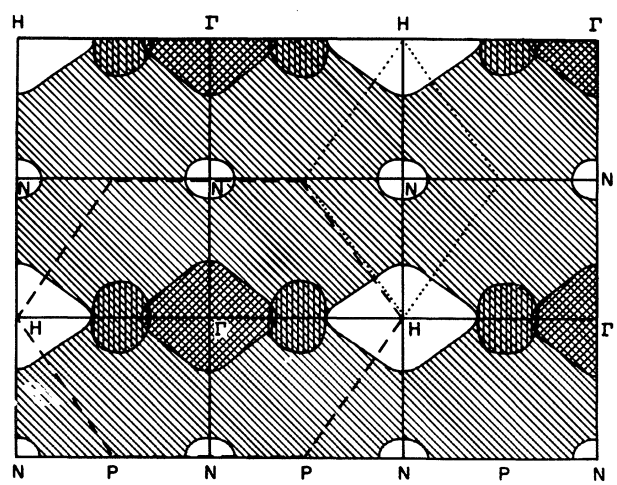

FIG. 1. A (110) section for the molybdenum Fermi surface as proposed by Lomer.