Random-field effects in site-disordered Ising antiferromagnets

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We describe a simple and unambiguous way of mapping the site-dilute Ising antiferromagnet in a uniform field onto the problem of a random-field ferromagnet, and identify the effective random field, in the weak-field limit.

Random-field Ising systems have attracted considerable recent theoretical and experimental attention. It was pointed out by Fishman and Aharony¹ that a dilute uniaxially anisotropic two-sublattice antiferromagnet in a uniform field gives a realization of such a system in that random local fields couple linearly to the antiferromagnetic order parameter. Since theoretical discussion has focused on the conceptually simpler ferromagnetic random-field model, it is important, for the antiferromagnet, to calculate the quantitative behavior of the effective random field H_{RF} in terms of the applied uniform field H.

In their original paper, Fishman and Aharony¹ considered bond disorder only. The antiferromagnetic order parameter was introduced by grouping the lattice sites into cells containing equal numbers of spins from each sublattice. However, the experimental systems considered²⁻⁴ actually exhibit substitutional site disorder, rather than bond disorder. Wong, von Molnar, and Dimon^{4,5} have extended the Fishman-Aharony argument to this case, using the same cell construction. They point out the existence of a "direct" random field, which is numerically larger than the Fishman-Aharony effect. This direct field would lead to a linear dependence of $H_{\rm RF}$ on H, even in strong applied fields.

Their explicit expression for the effective random field is somewhat complicated, and its calculation involves the detailed lattice structure. There are also several uncontrolled approximations, on which we shall comment at the end. In this paper we present an alternative expression for $H_{\rm RF}$ which is simple and easy to use in that it depends on only simple thermodynamic parameters of the system, and not the detailed microscopic Hamiltonian.

This approach involves performing a systematic Hubbard-Stratonovich⁶ transform from the discrete spin antiferromagnetic to a form in which the fluctuating degrees of freedom are the values of the local staggered magnetization $\phi(r)$. The random field is identified as the term coupling linearly to $\phi(r)$. Truncating this form at the Gaussian level corresponds exactly to solving the inhomogeneous meanfield equations. When higher-order terms are included we obtain the version which is the starting point for continuum analyses of the critical behavior of the random-field Ising model.^{7,8} These higher-order terms are irrelevant in the renormalization-group sense, and thus we establish that the dilute antiferromagnet is in the same universality class as the random-field ferromagnet, but they do, of course, affect nonuniversal properties by factors which are typically of order unity in the critical region.

We consider a simple site-dilute Ising antiferromagnet with Hamiltonian

$$\mathscr{H} = -\frac{1}{2} \sum_{r,r'} J(r-r') \epsilon(r) \epsilon(r') s(r) s(r') - H \sum_{r} \epsilon(r) s(r) .$$
(1)

Here $\epsilon(r) = 0$ or 1 depending on whether or not there is an impurity at site r. For definiteness we consider a discrete spin model with $s(r) = \pm 1$, although our main conclusions are valid for any good Ising-like system. The partition function $Z = \text{Tr}_s e^{-\beta \mathcal{X}}$ may be written, using the standard Hubbard-Stratonovich⁶ transformation, as

$$Z = \operatorname{Tr}_{\boldsymbol{\psi}} \operatorname{Tr}_{\boldsymbol{s}} \exp\left(-\frac{1}{2\beta} \sum_{\boldsymbol{r},\boldsymbol{r}'} \psi(\boldsymbol{r}) J^{-1}(\boldsymbol{r}-\boldsymbol{r}') \psi(\boldsymbol{r}') + \sum_{\boldsymbol{r}} [\beta H + \psi(\boldsymbol{r})] \epsilon(\boldsymbol{r}) s(\boldsymbol{r})\right)$$
(2)

$$= \operatorname{Trexp}_{\psi} \left\{ -\frac{1}{2\beta} \sum_{r,r'} \psi(r) J^{-1}(r-r') \psi(r') + \sum_{r} \epsilon(r) \ln \cosh[\beta H + \psi(r)] \right\} .$$
(3)

Here, $\psi(r)$ is a real scalar field. Note the fact that $\epsilon(r)$ may be factored out of the second term. This feature makes site disorder more tractable than bond disorder in this approach. Defining the local magnetization

$$M(r) = \beta^{-1} \sum_{r'} J^{-1}(r-r')\psi(r') ,$$

(3) may be rewritten as

$$Z = \operatorname{Tr}_{M(r)} \exp\left[-\frac{1}{2}\beta \sum_{r,r'} M(r)J(r-r')M(r') + \sum_{r'} \epsilon(r) \ln \cosh\beta\left[\sum_{r'} J(r-r')M(r') + H\right]\right] = \operatorname{Tr}_{M(r)} e^{-\beta F\{M\}} .$$
(4)

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The mean-field equations result from extremizing the exponent:

$$M(r) = \epsilon(r) \tanh\beta \left(\sum_{r'} J(r-r')M(r') + H \right)$$
(5)

$$= \epsilon(r) \tanh\beta \left(\sum_{r'} J(r-r') \epsilon(r') M(r') + H \right) .$$
(6)

The last equation follows because (5) implies that M(r) vanishes wherever $\epsilon(r)$ does. Equation (6) is the naive mean-field equation. Nevertheless, Eq. (4) correctly takes into account the fluctuations without an $\epsilon(r')$ factor present.

We expect the uniform magnetization to be nonzero in the presence of H, but its fluctuations to be noncritical. We therefore write

$$M(r) = M + (-1)'\phi(r) , \qquad (7)$$

where $(-1)^r$ is defined to be ± 1 on the two sublattices. *M* is chosen to satisfy the averaged mean-field equation

$$M = x \tanh\beta(\tilde{J}M + H) \quad , \tag{8}$$

where x is the concentration of magnetic ions $[\langle \epsilon(r) \rangle_{av} = x]$, and $\tilde{J} = \sum_{r} J(r)$. $\phi(r)$ is the antiferromagnetic order parameter. On substituting the decomposition (7) into the free-energy functional one finds a field h(r) coupling linearly to $\phi(r)$ of the form

$$h(r) = (-1)'\beta \left(-M\tilde{J} + \tanh\beta(\tilde{J}M + H) \sum_{r} J(r - r')\epsilon') \right)$$
(9)

$$= (-1)'\beta M \left[-\tilde{J} + x^{-1} \sum_{r'} J(r-r') \epsilon(r') \right] .$$
 (10)

Note that $\langle h(r) \rangle_{av} = 0$, as a consequence of *M* satisfying the mean-field equation. The correlations of h(r) are short ranged:

$$\langle h(r_1)h(r_2) \rangle_{av}$$

= $(-1)^{r_1-r_2} \frac{(1-x)\beta^2 M^2}{x} \sum_r J(r-r_1)J(r-r_2)$.

The full partition function has the form

$$Z = \operatorname{Tresp}_{\phi} \left\{ -\frac{1}{2}\beta \sum_{\mathbf{r},\mathbf{r}'} J(\mathbf{r}-\mathbf{r}')(-1)^{\mathbf{r}-\mathbf{r}'} \phi(\mathbf{r}) \phi(\mathbf{r}') + \sum_{\mathbf{r}} h(\mathbf{r}) \phi(\mathbf{r}) + \sum_{\mathbf{r}} \mu(\mathbf{r}) \phi(\mathbf{r})^{2} + \dots + \lambda \sum_{\mathbf{r}} \phi(\mathbf{r})^{4} + \dots \right\}.$$

This is precisely the starting point for the analysis⁶ of the continuous spin, random-field Ising model. There is also a random contribution to the ϕ^2 term corresponding to bond disorder. The mean-field transition temperature (at which the coefficient of ϕ^2 vanishes) is depressed according to

$$T_N^{\rm MF} = x \left[1 - (M/x)^2 \right] \overline{J} \quad , \tag{13}$$

where $\overline{J} = \sum_{r} (-1)^{r} J(r)$ is the mean-field transition temperature for the pure system, in the absence of a field.

The effective random field $h_{\rm RF}$ is best measured in terms

of the zero-momentum component of (11):

$$\langle h_{\rm RF}^2 \rangle_{\rm av} = \sum_{r_2} \langle h(r_1)h(r_2) \rangle_{\rm av} = \frac{x(1-x)(\beta \bar{J})^2(\beta H)^2}{(1-x\beta \bar{J})^2},$$
(14)

where we have solved the mean-field equation (8) for small H. This may be written in a more useful form

$$\langle h_{\rm RF}^2 \rangle_{\rm av} = \frac{x (1-x) [T_N^{\rm MF}(0)/T]^2 (H/k_B T)^2}{[1+\theta^{\rm MF}(x)/T]^2} ,$$
 (15)

which can be shown to be valid for a general spin-S Ising model. Here $k_B \theta^{MF} = \tilde{J}$ for the $S = \frac{1}{2}$ model, and, in general, is the usual parameter appearing in the Curie-Weiss susceptibility.

Equation (15) is our main result.⁹ If T_N^{MF} and θ^{MF} are replaced by their true values (a modification which is consistent with the other approximations) we have a simple compact formula which depends only on easily determined macroscopic parameters of the system. The approximation of dropping higher-order terms does not affect universal behavior, and should affect nonuniversal quantities by factors of order unity.

Our expression is in qualitative agreement with the corrected version of Wong *et al.*⁵ in the region to which it applies. The result obtained by formally setting $\theta_{MF} = 0$ in (15) corresponds precisely to the direct random field. The factor of $[T_N^{MF}(0)/T]^2 = (\beta \overline{J})^2$ is present because h_{RF} couples to the local staggered magnetization $\phi(r)$, rather than the original spins s(r). The full denominator in (15) reflects a modification of the direct random field by exchange effects, which act to reduce h_{RF} if the interaction is dominantly antiferromagnetic, i.e., $\theta^{MF} > 0$. For antiferromagnets with dominantly intersublattice exchange, $\theta^{MF} \approx T_N^{MF}$, and $\langle h_{RF}^2 \rangle$ is thus reduced by a factor of 4.

The additional factor $[T_N^{MF}(0)/T]^2$ leads to an overall x dependence in h_{RF}^2 at the critical point of the form (1-x)/x, since $T_N(x) \propto x$ for small x. Crossover theory¹ implies a fractional shift in the specific-heat peak, in a weak field H, proportional to

$$\langle (h_{\rm RF}^2) \rangle_{\rm av}^{1/\gamma} \propto [(1-x)H^2/x]^{1/\gamma}$$

This predicted x dependence is observed experimentally.¹⁰

The expression (15) differs in detail from that of Wong et al.⁵ This is because the approximations made are different. Their approach starts from the same Hamiltonian (1), and involves dividing the lattice into two-spin cells (a procedure which violates some lattice symmetries). Local ferromagnetic and antiferromagnetic order parameters are defined by $s_{\pm} = (s_1 \pm s_2)/\sqrt{2}$, where s_1 and s_2 are spins in one cell, on different sublattices. The Hamiltonian, which is quadratic in the s(r), is then written in terms of s_{+} and s_{-} , which are then treated as independent variables. This is exact if the s(r) are continuous Gaussian spins, but in the physical case when $s(r)^2 = 1$, there are infinitely strong correlations between s_+ and s_- . If this constraint is incorporated by including a term, for example, $\lambda \sum_{r} [s(r)^2 - 1]^2$, in the Hamiltonian, with $\lambda \rightarrow \infty$, the higher-order quartic terms give contributions to the effective random field, of $O(\lambda)$. We conclude that there may be large corrections to the expression of Wong et al.⁵ due to the discreteness of the spins. The appearance of these higher-order corrections was recognized in the original paper of Fishman and Aharony.¹

Another feature of the $H_{\rm RF}$ defined by Wong *et al.* is that

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it couples linearly to s_- . However $\langle s_- \rangle$ is not the local staggered magnetization, since s_- contains contributions from fictitious spins s(r) on the vacancies. Thus the true local order parameter is $x \langle s_- \rangle$. Thus their expression for $H_{\rm RF}$ should be divided by x to give the true random field to be used, for example, in the crossover theory. With this modification, the x dependence, at least of their direct term, agrees with that of our full expression, close to $T_N(x)$.

Finally, we note that our result (15) is valid only at weak fields $H \ll J$. For large H the truncation of the higher terms is not allowed. The effective random field H_{RF} acting on an equivalent *discrete* spin ferromagnet may be found by performing the same Hubbard-Stratonovich transformation and comparing the result with (12). In the large H limit, this leads to the direct random-field result $H_{RF} \propto H$, as expected.

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In conclusion, we have presented a theory of randomfield effects in site-dilute antiferromagnets which gives a simple form for the effective random field in weak applied fields, and a qualitative dependence on concentration which appears to agree with experiment. At the present time it is unlikely that experiment can distinguish between our form and that of Ref. 5, when correctly interpreted as discussed above.

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