observation of field-enhanced doping.[12] Again, the change is the response to a shift in the Fermi energy and can be explained on the basis of the $8-N$ rule as before.

From these examples I propose that an incipient photostructural instability is a universal property of any photoconductive amorphous semiconductor simply because the stable structure is a function of the position of E_F. The extent to which the instability is realized depends on the details of the relaxation and local reconstruction, which cannot be addressed here, and which will differ from one material to another.

In summary, I suggest that the position of E_F plays a determining role in the density and structure of localized states in a-Si:H. Substitutional doping can occur within the context of the $8-N$ rule but with limitations to the doping process which distinguish the doping of amorphous semiconductors from that of crystals. The present model emphasizes that both the doping efficiency and the defect density vary with the impurity concentration. An extension of these ideas to explain some nonequilibrium phenomena in a-Si:H is also suggested.

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Spin-Glass with Local Uniaxial Anisotropy

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A Heisenberg spin-glass with local uniaxial anisotropy is studied within replica mean-field theory, including consideration of replica-symmetry breaking. It is shown that it represents a very rich model with much to offer as a test bed for comparison of theory and experiment. The explanation of recent experiments on *Zn*Mn, *Mg*Mn, and *Cd*Mn is one of its consequences.

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The spin-glass[1] remains one of the more enigmatic unsolved problems of modern solid-state physics, having aspects quite contrary to those of conventional physics; such as an apparent practical breakdown of ergodicity, signaled by dramatic history dependence. However, for isotropic spin-glasses there has emerged a folklore of connections between experimental consequences and theoretical "fingerprints" in replica mean-field theory, a theoretical treatment in which the physical disordered system is mapped into an effective pure one involving replicated spins interacting through more complicated interactions and then analyzed in terms of a sophisticated mean-field theory.

In conventional pure systems with short-ranged interactions mean-field theory is at best approximate and may predict transitions in situations where fluctuations remove these transitions. By contrast, for spin-glasses the replica mean-field predictions are in reasonable qualitative accord with experiment while numerically exact evaluations[2] of Gibbs thermodynamic functions for short-range models in dimensions three or less indicate, contrary to observation, that there should be no transition. A complete understanding of the basis for this unusual correlation is not yet available, although it is believed to lie in the existence of a great range of time scales.[3] In the meantime, the replica mean-field theory is our best guide to experimental observation. The purpose of this Letter is to extend the theory to a vector spin-glass in the presence of uniform local uniaxial anisotropy. We show that this yields a rich range of predictions against which to test and help to understand the folklore mapping. It provides an explanation of recent experiments[4] on dilute alloys of Mn in Zn, Mg, and Cd and suggests several extensions of those experiments.

We restrict analysis to classical Heisenberg spins and mean-field theory, employing the infinite-range model for which the latter is believed to be exact. Explicitly, our Hamiltonian is[5]

$$\mathcal{H} = -\sum_{(ij)} J_{ij}\vec{S}_i\cdot\vec{S}_j - D\sum_i S_{iz}^2 - \sum_i \vec{H}\cdot\vec{S}_i,$$

where the J_{ij} are quenched random exchanges distributed with mean J_0/N and variance $J/N^{1/2}$. Units are chosen with spin lengths $\sqrt{3}$ and $J=k_B=1$, so that for $J_0=D=H=0$ the spin-glass transition is at $T=1$. D is allowed any magnitude or sign. The limiting models are (i) $D\to\infty$, Ising; (ii) $D\to-\infty$, planar xy; (iii) $D=0$, Heisenberg.

The analysis used is an extension of normal replica theory[6-8] including consideration of replica-symmetry breaking.[8,9] The solution is given in terms of self-consistently determined order parameters

$$m_\mu{}^\alpha = \lim_{n\to 0}\langle S_\mu{}^\alpha\rangle_n;\quad q_{\mu\nu}{}^{(\alpha\beta)} = \lim_{n\to 0}\langle S_\mu{}^\alpha S_\nu{}^\beta\rangle_n$$

where α,β label replicas; μ,ν label Cartesian directions. In replica-symmetric approximation $m_\mu{}^\alpha$ and $q_{\mu\nu}{}^{\alpha\beta}$ are independent of α and $q_{\mu\nu}{}^{(\alpha\beta)}$ with $\alpha\neq\beta$ are independent of $(\alpha\beta)$. For H along a Cartesian axis, only $q_{\mu\nu}$ with $\mu=\nu$ are nonzero. Replica-symmetry breaking is signaled by the softening of fluctuations in replica space around the symmetric solution. Within conventional folklore it is associated with the onset of history dependence.

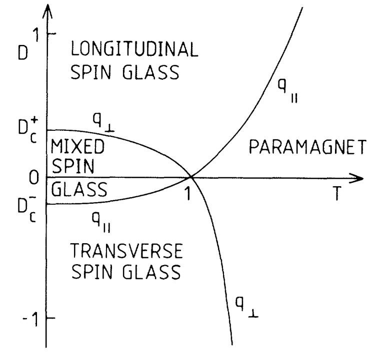

FIG. 1. Schematic phase diagram for a Heisenberg spin-glass with uniaxial local anisotropy; $J_0=0$, $J=1$, $S=\sqrt{3}$, $k_B=1$. The lines indicate $q_\parallel, q_\perp$-ordering transitions in replica-symmetric approximation with no external field. As $D\to\infty$, the $q_\parallel$-transition line is asymptotic to $T=3$; for $D\to-\infty$, the $q_\perp$-transition line is asymptotic to $T=\frac{3}{2}$.

Let us consider first the case $J_0=H=0$. Replica-symmetric theory can be parametrized via

$$q_\mu{}^\alpha = \langle\langle S_{i\mu}{}^2\rangle\rangle_d = 1 + (3\delta_{\mu,z}-1)x,$$

$$q_{\mu\mu}{}^{(\alpha\beta)} = q_\mu = \langle\langle S_{i\mu}\rangle^2\rangle_d = q_\perp + (q_\parallel - q_\perp)\delta_{\mu,z},$$

where $\langle\cdots\rangle$ and $\langle\cdots\rangle_n$ denote, respectively, thermodynamic averages over the real and the replicated systems, while $\langle\cdots\rangle_d$ denotes a quenched disorder average. Self-consistent equations for x and q_μ follow from the methods of Ref. 8:

$$q_\mu = (2\pi)^{-3/2}\iiint d^3t\,\exp(-t^2/2)(Z^{-1}\partial Z/\partial a_\mu)^2,\quad (1+2x) = (2\pi)^{-3/2}\iiint d^3t\,\exp(-t^2/2)(Z^{-1}\partial^2 Z/\partial a_z{}^2),$$

where

$$Z = \int_{-\sqrt{3}}^{\sqrt{3}} dS\,\exp(a_z S + bS^2) I_0((3-S^2)^{1/2}(a_x{}^2 + a_y{}^2)^{1/2}),\quad a_\mu = \beta t_\mu (q_\mu)^{1/2},\quad b = \beta D + \tfrac{1}{2}\beta^2(3x + q_\perp - q_\parallel).$$

$I_0(z)$ is a modified Bessel function of the first kind.

The resultant phase diagram is sketched in Fig. 1. For all D there is at least one spin-glass phase, longitudinal ($q_\parallel\neq 0$, $q_\perp=0$) for $D>0$ and transverse ($q_\perp\neq 0$, $q_\parallel=0$) for $D<0$. For $D_c{}^+ > D > D_c{}^-$ there is also a lower-temperature mixed spin-glass phase with both $q_\parallel$ and $q_\perp$ nonzero, but not isotropic (except for $D=0$). $D_c{}^\pm$ are estimated as 0.323 and -0.201, respectively. There is no phase transition associated with the quadrupolar parameter x.

Explicitly, the phase lines are given by the following. (i) $D>0$, *paramagnet–longitudinal spin-glass:*

$$T_{c1} = K_2(x_{c1})/K_0(x_{c1}),$$

where

$$K_n(x) = \int_{-\sqrt{3}}^{\sqrt{3}} dS\, S^n \exp[(\beta D + \beta^2 x)S], \quad x_{c1} = (T_{c1} - 1)/2.$$

(ii) $D < 0$, *paramagnet–transverse spin-glass:*

$$T_{c2} = [3 - K_2(x_{c2})/K_0(x_{c2})]/2,$$

where

$$x_{c2} = (1 - T_{c2}).$$

(iii) $D_c^+ > D > 0$, *longitudinal-mixed spin-glass:*

$$T_{c3} = \tfrac{1}{2}\{\int_{-\infty}^{\infty} [dt_z/(2\pi)^{1/2}] \exp(-t_z^2/2)[3 - J_2(\beta_{c3})/J_0(\beta_{c3})]\}^{1/2},$$

where

$$J_n(\beta) = \int_{-\sqrt{3}}^{\sqrt{3}} dS\, S^n \exp(a_z S + bS^2),$$

$q_\perp$ is zero, and x and $q_\parallel$ are determined throughout the longitudinal spin-glass phase by

$$1 + 2x = \int_{-\infty}^{\infty} [dt_z/(2\pi)^{1/2}] \exp(-t_z^2/2) J_2(\beta)/J_0(\beta), \quad q_\parallel = \int_{-\infty}^{\infty} [dt_z/(2\pi)^{1/2}] \exp(-t_z^2/2)[J_1(\beta)/J_0(\beta)]^2.$$

(iv) $0 > D > D_c^-$, *transverse-mixed spin-glass:*

$$T_{c4} = \{\iint_{-\infty}^{\infty} (dt_x dt_y/2\pi) \exp[-(t_x^2 + t_y^2)/2][H_2(\beta_{c4})/H_0(\beta_{c4})]^2\}^{1/2},$$

where

$$H_n(\beta) = \int_{-\sqrt{3}}^{\sqrt{3}} dS \exp(bS^2) S^n I_n((3 - S^2)^{1/2}(a_x^2 + a_y^2)^{1/2}),$$

$q_\parallel$ is zero, and x and $q_\perp$ are determined throughout the transverse spin-glass phase by

$$1 + 2x = \iint_{-\infty}^{\infty} (dt_x dt_y/2\pi) \exp[-(t_x^2 + t_y^2)/2] H_2(\beta)/H_0(\beta),$$

$$q_\perp = \iint_{-\infty}^{\infty} (dt_x dt_y/2\pi) \exp[-(t_x^2 + t_y^2)/2][G(\beta)/H_0(\beta)]^2,$$

with

$$G(\beta) = \int_{-\sqrt{3}}^{\sqrt{3}} dS \exp(bS^2) I_1((3 - S^2)^{1/2}(a_x^2 + a_y^2)^{1/2})(3 - S^2)^{1/2} t_x (t_x^2 + t_y^2)^{-1/2}.$$

Interreplica normal-mode analysis[8,9] shows that in fact replica symmetry is broken as soon as we enter a spin-glass phase; i.e., on $T_{c1}(D)$ for $D > 0$, on $T_{c2}(D)$ for $D < 0$. Once replica symmetry is broken, analytic calculation becomes more difficult and we lack a rigorously proven method. Parisi[10] has indicated a direction to follow for the Ising model. Extension to the present problem[11] indicates that replica-symmetry breaking does not remove the lower phase transitions.[12]

Within replica-symmetric theory the zero-field susceptibilities are given by

$$\chi_{\mu\nu} = [1 + (3\delta_{\mu,z} - 1)x - q_\mu]\delta_{\mu\nu},$$

predicting a cusp in $\chi_{\mu\mu}$ at the q_μ-ordering transition. Within the Parisi-type theory the replica-symmetric q_μ are replaced by functions $q_\mu(x)$ with the thermodynamic and linear response susceptibilities given by different measures over $q_\mu(x)$.[10,11] Again, however, q_μ-ordering transitions lead to discontinuities in the slopes of $\chi_{\mu\mu}(T)$. These predictions are in accord with the experiments of Albrecht *et al.*[4] who find (i) a spin-glass transition in the longitudinal direction alone for *Zn*Mn (34 and 62 ppm) for which they estimate $D/T_g(D)$[13] as 1.0 and 0.57, respectively, i.e., greater than our estimate of D_c^+; (ii) only a transverse spin-glass transition in *Cd*Mn (125 ppm) for which $D/T_g(D)$ is estimated as -1.15, i.e., less than D_c^-; (iii) apparently simultaneous longitudinal and transverse orderings for *Mg*Mn (186 and 274 ppm) for which $D/T_g(D)$ is estimated as 0.038 and 0.025, respectively, i.e., much smaller than $|D_c^\pm|$. Experimentally, D is local and to a first approximation concentration dependent, while the effective J is an increasing function of concentration.[14] Thus, increasing the Mn concentration would decrease the effective $|D|$ in our units (of J^{-1}) and it is a prediction of our theory that increasing the Mn concentration of *Zn*Mn or *Cd*Mn should lead to a second transition over and above those seen to date. Hexagonal rare-earth alloys would provide other experimental test beds.[15]

The inclusion of a magnetic field in the z direction makes $q_{\parallel}$ nonzero everywhere, rounds out the cusp in χ_{zz}, and reduces the $q_{\perp}$-ordering temperature. For D greater than a critical $D_c(H)$ there remains a sharp transition marking the onset of longitudinal replica-symmetry breaking, with $q_{\perp}$ still zero. $D_c(H)$ is the temperature at which the field-modified $q_{\perp}$-ordering and longitudinal replica-symmetry breaking transitions coincide. It is positive; for small H the reduction in the $q_{\perp}$-ordering temperature is proportional to H^2, and the longitudinal replica-symmetry breaking transition is reduced by order $H^{2/3}$. For $D < D_c(H)$, $q_{\perp}$ orders at a temperature higher than the continuation of the $D > D_c(H)$ longitudinal replica-symmetry breaking line and is itself accompanied by replica-symmetry breaking, dominantly transverse just below $T_{c2}(H)$, but everywhere with some longitudinal component. The detailed behavior of the $D < D_c(H)$ system near the continuation of the $D > D_c(H)$ longitudinal replica-symmetry breaking transition is presently unresolved, but it seems probable that it will be marked by a crossover in the longitudinal irreversibility.[8] This crossover will provide another of the tests alluded to earlier.

A field in the basal plane has more complicated mathematical consequences, but its physical effect is clear. A field in the x direction induces nonzero q_x but does not prevent q_y, q_z-ordering transitions. Replica symmetry breaks at these transitions with a lower-temperature crossover in the x irreversibility.

Detailed analysis of the effect of finite J_0 will also be deferred, but it is evident[7,14,16] that for $D > 0$ the replica-symmetry broken ($q_{\parallel} \neq 0$, $q_{\perp} = 0$, $H_z \neq 0$) phase maps into a replica-symmetry broken nonuniform collinear axial ferromagnet, and the ($q_{\parallel} \neq 0$, $q_{\perp} \neq 0$, $H_z \neq 0$) phase (for small enough D) maps into a replica-symmetry broken randomly canted axial ferromagnet, in each case for J_0 greater than a critical value. Related mappings to basal-plane ferromagnets exist for $D < 0$.

Finally, let us emphasize that our results are only for mean-field theory, but in view of the latter's success in simpler spin-glass models its extension is surely germane to unravelling the mystery of the spin-glass.

We thank P. Monod for drawing our attention to the work of Albrecht,[4] which stimulated this study, and D. J. Elderfield for help with computation. After the replica-symmetric work was complete, except for computation, the authors learned that a related study of the $J_0 = H = 0$ phase diagram had been undertaken by A. J. Bray and S. A. Roberts. They would like to thank these authors for a comparison of results for $D_c^{\pm}$. Financial assistance was provided by the Science and Engineering Research Council (United Kingdom).

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