

Interfaces (and Regional Congruence?) in Spin Glasses

C. M. Newman
Daniel L. Stein

SFI WORKING PAPER: 2001-03-019

SFI Working Papers contain accounts of scientific work of the author(s) and do not necessarily represent the views of the Santa Fe Institute. We accept papers intended for publication in peer-reviewed journals or proceedings volumes, but not papers that have already appeared in print. Except for papers by our external faculty, papers must be based on work done at SFI, inspired by an invited visit to or collaboration at SFI, or funded by an SFI grant.

©NOTICE: This working paper is included by permission of the contributing author(s) as a means to ensure timely distribution of the scholarly and technical work on a non-commercial basis. Copyright and all rights therein are maintained by the author(s). It is understood that all persons copying this information will adhere to the terms and constraints invoked by each author's copyright. These works may be reposted only with the explicit permission of the copyright holder.

www.santafe.edu



SANTA FE INSTITUTE

Interfaces (and Regional Congruence?) in Spin Glasses

C.M. Newman

Courant Inst. of Math. Sciences, New York Univ., New York, NY 10012

D.L. Stein

Departments of Physics and Mathematics, University of Arizona, Tucson, AZ 85721

Abstract

We present a general theorem restricting properties of interfaces between thermodynamic states and apply it to the spin glass excitations observed numerically by Krzakala-Martin and Palassini-Young in spatial dimensions $d = 3, 4$. We show that such excitations, with interface dimension $d_s < d$, *cannot* yield regionally congruent thermodynamic states. More generally, zero density interfaces of translation-covariant excitations cannot be pinned (by the disorder) in any d but rather must deflect to infinity in the thermodynamic limit. Additional consequences concerning regional congruence in spin glasses and other systems are discussed.

75.10.Nr, 05.70.Jk, 75.50.Lk, 75.40.Mg

Recent numerical studies [1–4] on finite-dimensional spin glasses observed unanticipated low-energy excitations that have generated considerable interest [5–8]. The models examined were nearest-neighbor Ising spin glasses with the Edwards-Anderson [9] Hamiltonian

$$\mathcal{H} = - \sum_{\langle x,y \rangle} J_{xy} \sigma_x \sigma_y , \quad (1)$$

where the couplings J_{xy} are independently chosen from a Gaussian distribution with mean zero and variance one, the sum is over only nearest neighbors on the d -dimensional cubic lattice, and the spins $\sigma_z = \pm 1$.

These studies examined the ground states $\pm\sigma^L$ and their low-energy excitations corresponding to the coupling realization \mathcal{J}^L inside cubes Λ_L of side L , centered at the origin, with periodic boundary conditions. Krzakala and Martin (KM) [1], working in $d = 3$, forced a random pair of spins, $\sigma_z, \sigma_{z'}$, to assume a relative orientation opposite to the one in σ^L , and then relaxed the rest of the spins to a new lowest-energy configuration. This ensures that at least some bonds in the excited spin configuration, σ'^L , must be changed (i.e., satisfied \leftrightarrow unsatisfied) from σ^L . It also ensures that the energy of σ'^L is no more than $O(1)$ above that of σ^L , regardless of L . Interestingly, rather than simply generating local droplet flips, the KM procedure was observed to yield large-scale (i.e., of lengthscale $l = O(L)$) excitations σ'^L , with $O(L^d)$ spins flipped from $\pm\sigma^L$, whose interface with σ^L (i.e., the set of bonds satisfied in σ'^L but not in σ^L , or vice-versa) had the property that the number of interface bonds scaled as L^{d_s} , with $d_s < d$.

Palassini and Young (PY) [2], working in both $d = 3$ and 4, excited σ^L differently by adding a novel coupling-dependent bulk perturbation to the Hamiltonian (1) in Λ_L . PY also interpreted their results as evidence of an excited σ'^L with $d_s < d$. At the same time the interface energy scaled as $l^{\theta'}$ ($\sim L^{\theta'}$), with $\theta' = 0$ [10]; i.e., it remains finite as $l \rightarrow \infty$ (presuming that l continues to grow as $O(L)$).

It is generally agreed [4] that the excitations of KM and of PY correspond to the same physical objects. We hereafter refer to them as *KMPY excitations*. Given a ground state σ^L (or ground state pair $\pm\sigma^L$) in Λ_L with coupling-independent boundary conditions (such

as periodic), KMPY excitations are global spin excitations whose structural and energetic properties scale with their length in a unique manner. More precisely, they are excitations σ'^L that are characterized by three properties: 1) they have $O(L^d)$ spins flipped from $\pm\sigma^L$ (and thus also have lengthscale $l = O(L)$); 2) the dimension d_s of their interface with σ^L satisfies $d_s < d$; and 3) their energy difference with σ^L (i.e., the interface energy) scales as $l^{\theta'}$ with $\theta' = 0$; i.e., the excitation energy remains of order one independently of l (and L).

Questions have been raised over the correct interpretation of these numerical results [5], and correspondingly whether KMPY excitations really exist in the spin glass phase [6,7]. We do not address these questions here. Rather, we take the point of view that if KMPY excitations *do* exist, then their physical meaning and implications for the low-temperature spin glass phase could be fundamentally important in the physics of disordered systems.

However, given the recentness of the discovery of KMPY excitations, their physical meaning and relevance remain unclear. By showing here rigorously that their interfaces *cannot* be pinned by the quenched disorder, we conclude that they cannot yield new ground or pure states. Such restrictions on their large-scale structure clarify the physical role they might play at low temperature T and provide general results on a type of ground and/or pure state multiplicity not heretofore investigated: the possibility in spin glasses of *regional congruence* [11] (see below).

Pinning. A crucial question about a new type of excitation is whether its boundary is *pinned*. This has not yet been addressed for KMPY interfaces, to our knowledge.

To understand pinning in this context, consider at $T = 0$ an increasing sequence of Λ_L 's. For each L , use the procedures of [1] or [2] to create KMPY excitations; e.g. [2], first generate the periodic boundary condition ground state σ^L , and then add a bulk perturbation (Eq. (2) of [2]) to the Hamiltonian to generate σ'^L , a perturbed ground state (i.e., an excited state for the original Hamiltonian). Then study the bonds $\langle x, y \rangle$ that obey

$$\sigma_x^L \sigma_y^L = -\sigma_x'^L \sigma_y'^L, \quad (2)$$

i.e., those that are satisfied in one state but not the other. The corresponding set of bonds

in the dual lattice comprises the finite-size “domain wall” (for that L) or interface of the excitation (i.e., the boundary of the set of spins that are flipped to go from σ^L to σ'^L).

By pinning we mean the following. Consider a fixed L_0 (which can be arbitrarily large). Apply the KM or PY procedure on cubes Λ_L , with $L \gg L_0$. Observe $\sigma'^{(L,L_0)}$, the excited spin configuration σ'^L restricted to Λ_{L_0} . If the excitation interface remains inside Λ_{L_0} as $L \rightarrow \infty$ [12], then the interface is *pinned*.

If the interface is *not* pinned, we say it “deflects to infinity”. Here, for any fixed L_0 , the interface, for all L above some L' , will *not* enter Λ_{L_0} . (This is what occurs with interface ground states in disordered ferromagnets for small d [13–15].) See Fig. 1 for a schematic illustration.

FIGURES

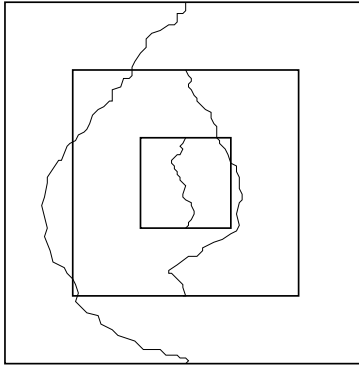


FIG. 1. A sketch of interface deflection to infinity for $d = 2$. As L increases, the interface recedes from the origin. The interfaces eventually are completely outside any fixed square. (The deflection can scale more slowly with L than in the figure.)

Scenarios. Assuming now that KMPY excitations do exist on at least small to moderate lengthscales, there are four possibilities for larger lengthscales. One is that the excitations disappear altogether, noted as a possibility in [2]. Of the three remaining (more interesting) scenarios, two have the KMPY interface pinned, and the third has it deflect to infinity.

Scenario (1): KMPY excitations are pinned and give rise to new ground states at $T = 0$ and new pure states at $T > 0$ (below some T_c). I.e., their interfaces with the original ground state, or with each other, become relative domain walls between distinct ground (or pure) states not related by a global spin flip. (For more details on relative domain walls, see [16,17].) This interesting picture differs from previous proposals for the low- T spin glass phase, and would be the first example of *regional congruence* [11] in spin glasses. Two distinct thermodynamic states that are not global flips of each other are regionally congruent if the total relative domain wall density vanishes; i.e., essentially the condition above that $d_s < d$. (If the density is nonzero so that $d_s = d$, as is more usually supposed, the states are said to be *incongruent*.)

Scenario (2): The excitations are pinned, but do *not* give rise to new ground states. For this to occur, any $L \rightarrow \infty$ limit of σ^L must be energetically unstable (in the Hamiltonian (1)) to the flip of some fixed *finite* droplet. Even if this occurs, it could be that KMPY

excitations, at $T > 0$, still give rise to new *pure* states.

Scenario (3): KMPY excitations persist on all lengthscales, but their interfaces deflect to infinity, as in Fig. 1. If this occurs, they cannot give rise to new thermodynamic ground or pure states, but could still be relevant to the excitation spectrum in finite volumes.

Which of these scenarios actually occurs was not addressed in [2], although [3] as well as [8] implicitly or explicitly assume Scenario (1). Determining which occurs is crucial to understanding the role of these excitations in the spin glass phase.

We now prove that *KMPY excitations cannot be pinned by the quenched disorder, ruling out Scenarios (1) and (2)*. (A heuristic argument against Scenario (1) was presented in [18].) The remaining possibility (in which KMPY excitations persist on all lengthscales) is Scenario (3), where they deflect to infinity. Before presenting our theorem, we introduce the concept of *metastate*, which is implicit in the theorem and useful for understanding its applications.

Metastates. A ($T = 0$) metastate gives the probability of finding various ground state pairs in typical large volumes. There are different constructions (technical details are in [16,19–21]); we give here only a simple physical description.

Consider the cube Λ_{L_0} with (large) fixed L_0 , and then examine a sequence of Λ_L 's with $L \rightarrow \infty$, all with (for example) periodic boundary conditions. Look, for each L , at the part of the ground state σ^L inside the smaller fixed Λ_{L_0} , and keep a record of the fractions of L 's in which different spin configurations appear inside Λ_{L_0} . (If there's only a single pair of thermodynamic ground states, then one eventually sees one fixed configuration inside Λ_{L_0} , and thus asymptotically the ground state pair appears inside Λ_{L_0} for a fraction one of the L 's). The resulting ($T = 0$, periodic boundary condition) metastate is a probability measure on infinite-volume ground state pairs that provides information on the fraction of L 's for which each of them appears inside Λ_{L_0} .

For the coming theorem, we extend the notion of metastate to *uniform perturbation metastate* [22]. For each L , consider, in addition to σ^L , a second σ'^L (which in practice will be the ground state of a perturbed Hamiltonian) chosen so as to respect the finite-volume

(torus) translation-invariance already present for $(\mathcal{J}^L, \sigma^L)$ due to the periodic boundary conditions. (We show later that this holds for σ'^L in both KM and PY constructions.) Then do for the *pair* (σ^L, σ'^L) what was done for σ^L in the original metastate. The resulting uniform perturbation metastate gives for both (infinite-volume) ground and excited states their relative frequency of appearance inside large volumes. The theorem presents implications of translation-invariance on the resulting interfaces, and shows that if there is a (pinned) interface at all, it must have strictly positive density (so $d_s = d$).

Theorem. On the cube Λ_L with periodic boundary conditions, for a given coupling configuration \mathcal{J}^L let σ^L and σ'^L be a pair of spin configurations such that the joint distribution of $(\mathcal{J}^L, \sigma^L, \sigma'^L)$ is invariant under (torus) translations of Λ_L . Let $(\mathcal{J}, \sigma, \sigma')$ be any limit in distribution as $L \rightarrow \infty$ of $(\mathcal{J}^L, \sigma^L, \sigma'^L)$. Then for almost every $(\mathcal{J}, \sigma, \sigma')$ either $\sigma' = \pm\sigma$ or else σ and σ' have a relative interface of strictly positive density.

Proof. Because the joint distribution κ^L of $(\mathcal{J}^L, \sigma^L, \sigma'^L)$ is for every L invariant under torus translations, any limiting distribution κ of $(\mathcal{J}, \sigma, \sigma')$ is invariant under all translations of the infinite-volume cubic lattice. The translation-invariance of κ allows its decomposition into components in which translation-ergodicity holds (see, e.g., [21,23]). For each bond $\langle x, y \rangle$ consider the event $A_{\langle x, y \rangle}$ that $\langle x, y \rangle$ is satisfied in one but not the other of σ, σ' . In each ergodic component, either the probability of $A_{\langle x, y \rangle}$ equals zero and then there is no interface (i.e., $\sigma' = \pm\sigma$) or else it equals some $\rho > 0$. In the latter case, by the spatial ergodic theorem (see, e.g., [21,23]) the spatial density of $\langle x, y \rangle$'s such that $A_{\langle x, y \rangle}$ occurs must equal ρ , i.e., the (σ, σ') interface has a nonzero density. Thus there is zero probability (with respect to κ) of a $(\mathcal{J}, \sigma, \sigma')$ such that there is a σ, σ' interface, but with zero density.

Remarks. 1) If one takes the $\kappa(\mathcal{J}, \sigma, \sigma')$ of the theorem and conditions it on the coupling realization \mathcal{J} , the resulting conditional distribution $\kappa_{\mathcal{J}}(\sigma, \sigma')$ is the uniform perturbation metastate discussed above. Equivalent to the theorem's conclusion is that for almost every \mathcal{J} , if σ and σ' are chosen from $\kappa_{\mathcal{J}}(\sigma, \sigma')$, there is zero $\kappa_{\mathcal{J}}$ -probability of an (infinite-volume) interface with zero density. This rules out (σ^L, σ'^L) interfaces with $d_s < d$ that are also

pinned.

2) Although the theorem as formulated here addresses ground and excited states at $T = 0$, it should be extendable to pure states at (low) $T > 0$ by “pruning” small thermally induced droplets.

3) Although our construction used periodic boundary conditions (both for simplicity and because KM and PY used them), the theorem can be applied to other boundary conditions chosen independently of the couplings (as in [17], to which we refer the reader for details).

4) Although our focus here is on spin glasses, the theorem applies equally to many other systems, including disordered and homogeneous ferromagnets.

Application to KMPY excitations. An immediate application of the theorem is that KMPY excitations cannot be pinned, and so cannot give rise to (regionally congruent) ground states. To see that the theorem applies to the PY construction, note first that the periodic boundary condition clearly implies torus translation invariance for the distribution of $(\mathcal{J}^L, \sigma^L)$. The Hamiltonian perturbation (Eq. (2) of [2]) is constructed from σ^L in a translation-covariant way, and thus the distribution of $(\mathcal{J}^L, \sigma^L, \sigma'^L)$ is also invariant.

A priori, the situation for the KM construction is more subtle. Here if σ'^L results from a *fixed* pair of spins at sites z_0, z'_0 , translation-invariance would be lost. So instead, for fixed \mathcal{J}^L and σ^L we regard σ'^L as the *random* excitation resulting when z, z' are chosen for each Λ_L from the uniform distribution on its sites; this restores translation-invariance. A first result is then that for a fraction one (as $L \rightarrow \infty$) of such choices of z, z' , the interface cannot be pinned. But there’s a second, more noteworthy result: it follows that a *fixed* z_0, z'_0 cannot yield a KMPY (or similar) excitation (which now would necessarily be pinned) at all, since if it did there would be a positive fraction of random (z, z') ’s yielding the same excitation. *Thus a fixed z_0, z'_0 must either yield a droplet excitation with volume $o(L^d)$ (e.g., bounded) as $L \rightarrow \infty$ or else one with $d_s = d$.*

Regional Congruence. As discussed above, regionally congruent thermodynamic states [11] are those whose relative interfaces have zero density. Examples are the interface states in homogeneous and disordered Ising ferromagnets for sufficiently large d . But prior to [1]

and [2] there had been no evidence for the existence of regional congruence in spin glasses.

In [16] and [17], we proved that thermodynamic states generated by coupling-independent boundary conditions (e.g., periodic, antiperiodic, free, fixed, etc.) are (with probability one) either the same (modulo a global spin flip) or else incongruent (so $d_s = d$). Thus regionally congruent states can *only* arise, if at all, through a sequence of Λ_L 's with *coupling-dependent* boundary conditions; i.e., those that are *conditioned* on the \mathcal{J}^L 's. This is consistent with the above theorem, because such boundary conditions typically violate translation-invariance. E.g., interface states in ferromagnets arise through boundary conditions, such as Dobrushin [24,25] (i.e., plus boundary spins above the “equator” and minus below), that are not translation-covariant and implicitly use the knowledge that all couplings are positive. But in a spin glass, they are now gauge-equivalent to boundary conditions that *are* both translation-covariant and coupling-*independent*.

But now conclusions beyond those of [16,17] follow from the theorem, because in addition regional congruence cannot arise through any translation-covariant construction. A consequence is that any algorithm of the types currently known *cannot* yield regionally congruent states. The KM and PY procedures typify two main approaches in the search for new excitations and/or states, given that *a priori* the interface location is unknown: either a uniformly random sampling procedure (KM) or else a global perturbation (PY) (or similar coupling to a carefully chosen external field). Although the latter approach *is* coupling-dependent, it is also translation-covariant and so cannot generate regional congruence. One method that *could* find regional congruence, if it occurs, is an exhaustive search through all $2^{O(L^{d-1})}$ fixed boundary conditions on Λ_L for each L ; but that is hardly an option.

We conclude by noting that the order one energy difference of σ, σ' plays no role in our theorem, which in fact has far wider applicability. Only *one* of its applications is to KMPY excitations, but these have generated interest *because* both $\theta' = 0$ and $d_s < d$. However, the order one energy does play a crucial role in our earlier heuristic argument [18], which we briefly summarize (and slightly extend) here. It was conjectured [26] and subsequently proved [27] (also [28]) that free energy fluctuations in spin glasses with coupling-independent

boundary conditions on Λ_L scale as L^θ , with $\theta \leq (d-1)/2$. It should then follow that the exponent θ_r characterizing interface energies for regionally congruent states satisfies the bound $\theta_r > \theta$ (as argued in [28–30]) because otherwise regional congruence could be seen with coupling-independent boundary conditions. So pinned interfaces with $d_s < d$ (hence regionally congruent states) must have $\theta_r > \theta$; if the latter inequality is violated, as in KMPY excitations, then the interface should deflect to infinity.

Acknowledgments. This research was supported in part by NSF Grants DMS-98-02310 (CMN) and DMS-98-02153 (DLS). The authors thank Peter Young and Matteo Palassini for useful correspondence. They also thank the Santa Fe Institute, where part of this work was done, for its hospitality.

REFERENCES

- [1] F. Krzakala and O.C. Martin, Phys. Rev. Lett. **85**, 3013 (2000). Also available as cond-mat/0002055.
- [2] M. Palassini and A.P. Young, Phys. Rev. Lett. **85**, 3017 (2000). Also available as cond-mat/0002134.
- [3] J. Houdayer, F. Krzakalam and O.C. Martin, available as cond-mat/0009382.
- [4] H.G. Katzgraber, M. Palassini, and A.P. Young, available as cond-mat/0007113.
- [5] A.A. Middleton, available as cond-mat/0007375.
- [6] E. Marinari and G. Parisi, available as cond-mat/0005047.
- [7] E. Marinari and G. Parisi, available as cond-mat/0007493.
- [8] G. Hed, A.K. Hartmann, and E. Domany, available as cond-mat/0012451.
- [9] S.F. Edwards and P.W. Anderson J. Phys. F **5**, 965 (1975).
- [10] This is different from the exponent θ governing the energy change between coupling-independent boundary conditions, such as periodic to antiperiodic. Numerical studies in $d = 3, 4$ suggest $\theta > 0$ (see, e.g., D.S. Fisher and D.A. Huse, Phys. Rev. B **38**, 386 (1988)).
- [11] D.A. Huse and D.S. Fisher, J. Phys. A **20**, L997 (1987).
- [12] We require this only for *some* arbitrarily large L 's, but presumably it will then be true for all large L with the interface converging to a well-defined limit as $L \rightarrow \infty$.
- [13] D.A. Huse and C.L. Henley, Phys. Rev. Lett. **54**, 2708 (1985).
- [14] M. Kardar, Phys. Rev. Lett. **55**, 2923 (1985).
- [15] A. Bovier and C. Külske, Rev. Math. Phys. **6**, 413 (1994).

- [16] C.M. Newman and D.L. Stein, Phys. Rev. Lett. **84**, 3966 (2000).
- [17] C.M. Newman and D.L. Stein, available as cond-mat/0103395.
- [18] C.M. Newman and D.L. Stein, available as cond-mat/0010033.
- [19] M. Aizenman and J. Wehr, Commun. Math. Phys. **130**, 489 (1990).
- [20] C.M. Newman and D.L. Stein, Phys. Rev. Lett. **76**, 4821 (1996).
- [21] C.M. Newman and D.L. Stein, Phys. Rev. E **55**, 5194 (1997).
- [22] This is related to the *excitation metastate* of [17], but with the difference that here perturbations are applied in a uniform, translation-invariant manner.
- [23] C.M. Newman and D.L. Stein, Phys. Rev. Lett. **76**, 515 (1996).
- [24] R.L. Dobrushin, Theor. Prob. Appl. **17**, 582 (1972).
- [25] C.M. Newman and D.L. Stein, Phys. Rev. E **63**, 16101-1 (2001).
- [26] D.S. Fisher and D.A. Huse, Phys. Rev. Lett. **56**, 1601 (1986).
- [27] M. Aizenman and D.S. Fisher, unpublished.
- [28] C.M. Newman and D.L. Stein, Phys. Rev. B **46**, 973 (1992).
- [29] D.S. Fisher and D.A. Huse, J. Phys. A **20**, L1005 (1987).
- [30] A. van Enter, J. Stat. Phys. **60**, 275 (1990).