Proof of Single-Replica Equivalence in Short-Range Spin Glasses

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We consider short-range Ising spin glasses in equilibrium at infinite system size, and prove that, for fixed bond realization and a given Gibbs state drawn from a suitable metastate, each translation and locally invariant function (for example, self-overlaps) of a single pure state in the decomposition of the Gibbs state takes the same value for all the pure states in that Gibbs state. We describe several significant applications to spin glasses.

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The nature of the spin-glass (SG) phase in classical finite-dimensional short-range models remains one of the outstanding unsolved problems in statistical mechanics. Although important fundamental questions remain open, considerable analytical and numerical progress has been made, especially on the rigorous theory of mean-field SGs [1–8] and short-range SGs (for a recent review, see Ref. [9]). For the mean-field case, which corresponds to infinite-range models such as the Sherrington-Kirkpatrick (SK) Ising Hamiltonian [10], most of the fundamental problems have been solved by the replica symmetry-breaking (RSB) theory [11–15].

For the short-range case, in which we will focus on Ising spins ($s_{\mathbf{x}} = \pm 1$ for all sites $\mathbf{x}$) and infinite system size, there is an unresolved controversy about whether the low-temperature phase involves many ordered or "pure" states as in RSB, or only one or two, as in the scaling-droplet (SD) picture [16–19]. Rigorous results have been obtained using *metastates* [20–23]; a metastate is a probability distribution on equilibrium (i.e., Gibbs) states, with covariance properties we describe below. In the SD picture, the metastate is trivial (i.e., supported on a single Gibbs state), while for RSB behavior the metastate is necessarily nontrivial [9,21–26], and a Gibbs state in its support is a nontrivial mixture of many pure states (if there is global spin-flip symmetry under $s_{\mathbf{x}} \to -s_{\mathbf{x}}$ for all $\mathbf{x}$, these are not all related by symmetry).

In this Letter, we establish a further necessary property of pictures with Gibbs states that are nontrivial mixtures of pure states. Loosely, for systems *without* spin-flip invariance, there is no macroscopic order parameter that can distinguish between the pure states in a Gibbs state; i.e., for given bonds and Gibbs states (drawn from a metastate, which can be trivial or nontrivial), all pure states in the Gibbs state "look alike," in that each macroscopic property (defined precisely later) defined for any single pure state takes the same value in all the pure states. For example, all pure states in a given Gibbs state have the same self-overlap, magnetization, and internal energy density. Similarly, *with* spin-flip invariance, pure states cannot be distinguished from one another by *flip-invariant* order parameters (note that magnetization is not flip invariant). We call this property "single-replica equivalence." (A similar statement, that self-overlaps almost surely take a single value in *infinite*-range models, assuming that the Ghirlanda-Guerra identities [2] hold, was proved in Ref. [27].) This result has a number of immediate applications that we describe later. For technical reasons, the proof of our result is for models with interactions within groups of p spins, for all p (or all even p); the case of only nearest-neighbor pair interactions is not included, but it can be approached arbitrarily closely.

Single-replica equivalence is so named because of its similarity to replica equivalence [28]. Here the term "replica" refers to real replicas—i.e., pure states drawn from some distribution. Replica equivalence asserts that functions of overlaps of distinct replicas are independent of the choice of one of the replicas; this is not the property that we discuss, but it may possibly be related.

We now define notations and review concepts that will be needed in what follows. The sites $\mathbf{x}$ lie in the d-dimensional cubic lattice $\mathbb{Z}^d$, and we define $s = (s_{\mathbf{x}})_{\mathbf{x}\in\mathbb{Z}^d}$. Let X denote a nonempty finite set of distinct sites, $\mathcal{X}$ the set of all such X, and $s_X = \prod_{\mathbf{x}\in X} s_{\mathbf{x}}$. A general Hamiltonian is then

$$H_J(s) = -\sum_{X\in\mathcal{X}} J_X s_X, \tag{1}$$

where $J = (J_X)_{X\in\mathcal{X}}$ is an indexed set of independent random variables (bonds), one associated with each $X \in \mathcal{X}$, so the joint distribution $\nu(J)$ of J_X for all X is a translation-invariant product (over X) distribution; we write expectation under ν as $\mathbf{E}\cdots$. We define a "mixed p-spin model" of this form ("mixed" means the sum is over all $X \in \mathcal{X}$, and p denotes values of $|X|$) to be (I) "short range" if $\sum_{X:\mathbf{x}\in X} \mathbf{E}|J_X| < \infty$ for any $\mathbf{x}$ (see, e.g., Ref. [29]), and (II) "n.i.p." if, for every X such that $\mathrm{Var}J_X > 0$ (possibly infinite), there are *no isolated points* in the support of the marginal distribution for J_X [e.g., the marginal is continuous (i.e., atomless)]. For spin-flip invariance of H_J under $s \to -s \equiv (-s_\mathbf{x})_{\mathbf{x}\in\mathbb{Z}^d}$, we impose also (III) $J_X = 0$ for $|X|$ odd. The familiar EA Hamiltonian [30] is a special case of these models in which $J_X = 0$ if X is neither a nearest-neighbor pair nor a single site. For a SG, one typically assumes that J_X has mean zero (except possibly for $|X| = 1$, the single-site magnetic field terms), but the mean-zero assumption is neither required nor assumed in the theorems and proofs below.

States Γ [i.e., probability distributions $\Gamma(s)$ on configurations s] are uniquely determined by the values of the expectations $\langle s_X\rangle_\Gamma$ in Γ as X runs through $\mathcal{X}$. An (infinite-volume) Gibbs state is defined for a given short-range Hamiltonian, such as $H_J(s)$, and for fixed temperature T ($0 < T < \infty$) as a state that obeys the Dobrushin-Lanford-Ruelle conditions [31,32]. A convex combination (i.e., a mixture) of Gibbs states is again a Gibbs state.

A Gibbs state may be either pure or mixed. A pure state is a Gibbs state that is extremal—i.e., not expressible as a mixture of other Gibbs states. Equivalently, it obeys a strong clustering property [31,32] that implies the decay of connected correlations to zero. Distinct pure states put all their probability on disjoint sets of spin configurations [31,32]. We will denote pure states by Γ_α and expectation in Γ_α as $\langle\cdots\rangle_\alpha$ (α is an index). Any Gibbs state Γ can be expressed, or "decomposed," as a unique mixture of pure states [31]; that is,

$$\Gamma = \sum_\alpha w_\alpha \Gamma_\alpha \tag{2}$$

for a set of non-negative weights $w_\alpha = w_\Gamma(\alpha)$ that obey $\sum_\alpha w_\alpha = 1$ (i.e., probabilities) and which depend on J and Γ. Equation (2) corresponds to a countable decomposition, but our results hold in the general case, where every sum $\sum_\alpha w_\alpha\cdots$ with weights w_α becomes an integral $\int dw_\Gamma(\alpha)\cdots$ with probability measure $dw_\Gamma(\alpha)$. A spin-flip transformation sends any state Γ to a state $\bar\Gamma$, defined by $\bar\Gamma(s) = \Gamma(-s)$. $\bar\Gamma = \Gamma$ if and only if $\langle s_X\rangle_\Gamma = 0$ whenever $|X|$ is odd. Spin-flip symmetry of H_J implies that for each pure state Γ_α there is a flipped pure state $\Gamma_{\bar\alpha} = \overline{\Gamma_\alpha}$, and that for a flip-invariant Gibbs state we have $w_{\bar\alpha} = w_\alpha$ for all α.

Two other types of transformation will be important. The first type are translations: if all bonds in a given J are translated by a fixed amount, then the same translation applied to any Gibbs state Γ for J produces a corresponding Gibbs state for the translated J. The second type are local transformations: for any $\Delta J_X \neq 0$ for finitely many X, a state Γ transforms to a state Γ' defined by [20,33]

$$\langle\cdots\rangle_\Gamma \to \langle\cdots\rangle_{\Gamma'} = \frac{\langle\cdots e^{\beta\sum_X \Delta J_X s_X}\rangle_\Gamma}{\langle e^{\beta\sum_{X'} \Delta J_{X'} s_{X'}}\rangle_\Gamma}, \tag{3}$$

where $\beta = 1/T$. When Γ is a *pure* state Γ_α for H_J, the locally transformed state is a pure state Γ'_α for $H_{J+\Delta J}$, so we can use the same labels α.

More generally, states Γ and Γ' are related as in Eq. (3) and are Gibbs states for H_J and $H_{J+\Delta J}$, respectively, if and only if they are mixtures of pure states Γ_α, Γ'_α for the respective Hamiltonians with respective weights w_α, w'_α related by [20,33]

$$w'_\alpha = \frac{r_\alpha w_\alpha}{\sum_\gamma r_\gamma w_\gamma}, \tag{4}$$

where

$$r_\alpha = \langle e^{\beta\sum_X \Delta J_X s_X}\rangle_\alpha. \tag{5}$$

Our main objects of interest are *invariant observable properties* of pure states. We define an invariant observable $O(J, \Gamma_\alpha)$ to be a (Borel-measurable) function of (J, Γ_α) that is invariant under both translations and local transformations. When spin-flip symmetry is present, we consider local changes in J_X only for $|X|$ even, and we can consider observables that are also invariant under a spin-flip transformation of Γ_α.

Examples include translation averages of spin expectations. We define the translation of a site $\mathbf{x}$ by a vector $\mathbf{x}'$ to be $\tau_{\mathbf{x}'}\mathbf{x} = \mathbf{x} + \mathbf{x}'$; for a set $X = \{\mathbf{x}_i:\ i = 1, \ldots, p\}$ of sites, $\tau_{\mathbf{x}'}X$ is defined in the obvious way. Also, for W a positive odd integer, we define $\Lambda_W \subset \mathbb{Z}^d$ to be a hypercube of side $W - 1$, centered on the origin, so that $|\Lambda_W| = W^d$ sites. For a function f_X, its translation average $\mathrm{Av} f_X$ is

$$\mathrm{Av}\, f_X = \lim_{W\to\infty} \frac{1}{W^d} \sum_{\mathbf{x}'\in\Lambda_W} f_{\tau_{\mathbf{x}'}X}, \tag{6}$$

provided the limit exists.

Postponing the latter issue for a moment, some examples of invariant observables for a Γ_α are as follows: (i) The magnetization per site, $\mathrm{Av}\langle s_\mathbf{x}\rangle_\alpha$ (here $X = \{\mathbf{x}\}$ and $f_X = \langle s_\mathbf{x}\rangle_\alpha$), and generalizations to all s_X in place of a single spin $s_\mathbf{x}$. (ii) The EA single-site quadratic self-overlap $\mathrm{Av}\langle s_\mathbf{x}\rangle_\alpha^2$, the two-site or edge self-overlaps $\mathrm{Av}\langle s_\mathbf{x}s_\mathbf{y}\rangle_\alpha^2$ (for which $X = \{\mathbf{x}, \mathbf{y}\}$), and their generalizations to all s_X. (iii) More general forms, involving the overlaps of all degrees [of which (i) and (ii) are special cases],

$$\mathrm{Av}\prod_{i=1}^{n}\langle s_{X_i}\rangle_\alpha, \tag{7}$$

where X_i, $i = 1, \ldots, n$ are finite sets, $X = \cup_i X_i$, and the translation average is over simultaneous translations of all X_i. Spin-flip invariant examples include all those in (ii), and those in Eq. (7) if $\sum_i |X_i|$ is even.

Other examples are (iv) parts of the internal energy density, with $f_X = -J_X\langle s_X\rangle_\alpha$ for each X, and the internal energy density itself; and (v) the free energy density, and hence, using (iv), the entropy density also. All examples in (iv) and (v) are spin-flip invariant whenever H_J is.

To make further progress, we introduce metastates. A metastate $\kappa_J(\Gamma)$ is a probability distribution on states Γ for given J, such that a state drawn from it is a Gibbs state for J, with $\nu\kappa_J$ probability 1 [i.e., $\nu\kappa_J$–almost every (J, Γ)]; we write $\mathbf{E}_{\kappa_J}\cdots$ for the expectation under κ_J. Metastates were originally constructed to describe asymptotically large, finite-size systems in equilibrium [20–23]. They are particularly useful for systems with chaotic size dependence [34], which may prevent directly taking the thermodynamic limit with bond-independent boundary conditions (BCs). Metastates using periodic BCs in the finite-size systems are covariant under both translations and local transformations [20–23]. Covariance states that, if θ denotes either a translation or a local change of J, and also the corresponding transformation of a state Γ, then $\kappa_{\theta J}(\Gamma) = \kappa_J(\theta^{-1}\Gamma)$. That is, under a transformation of J of either type, the weight in κ_J flows to corresponding transformed Gibbs states. These properties are crucial in what follows.

For H_J with spin-flip symmetry, we require a metastate such that any Gibbs state drawn from it is spin-flip invariant. This is automatic when a spin-flip-invariant BC (e.g., periodic) is used in the construction.

To show invariance for an observable in cases (i)–(iv) above, we use translation invariance of ν, translation covariance of κ_J, and also translation covariance of $w_\Gamma(\alpha)$ under translations of (J, Γ), which follows from the translation property of Γ. Together these imply that the probability distribution $\nu(J)\kappa_J(\Gamma)w_\Gamma(\alpha)$ on J, Γ, and Γ_α is translation invariant. For any function f_X of J, Γ_α for given (J, Γ) such that $\mathbf{E}\mathbf{E}_{\kappa_J}\int dw_\Gamma(\alpha)|f_X| < \infty$, it follows directly from the ergodic theorem for translations [31] that $\mathrm{Av} f_X$ exists and is translation invariant, for $\nu\kappa_J w_\Gamma$–almost every $(J, \Gamma, \Gamma_\alpha)$. Invariance under local transformations then also holds, because the translation average involves a sum over $\mathbf{x}' \in \Lambda_W$, and by the clustering property of pure states, the change in each thermal average is arbitrarily small except for a fraction of $\mathbf{x}'$ values that tends to zero as $W \to \infty$. We discuss the free energy density after Theorem 1.

We can now formulate a full statement of our result:

Theorem 1.—Consider a short-range n.i.p. mixed p-spin model with $\mathrm{Var}J_X > 0$ for all $X \in \mathcal{X}$, and an invariant observable property $O(J, \Gamma_\alpha)$, where the pure state Γ_α appears in the decomposition [Eq. (2)] of a Gibbs state Γ drawn from a metastate κ_J, with J drawn from ν. Then, for ν–almost every J and κ_J–almost every Γ, $O(J, \Gamma_\alpha) = O(J, \Gamma_{\alpha'})$ for $w_\Gamma \times w_\Gamma$–almost every pair of pure states α, α' in the decomposition of Γ. In the spin-flip-invariant case, the conditions are the same except that $\mathrm{Var}J_X > 0$ for all $X \in \mathcal{X}$ with $|X|$ even; then the statement holds for invariant observables O that are spin-flip invariant.

Remarks.—(a) We emphasize that the result does not say that the invariant observable takes the same value in pure states in the decomposition of *different* Gibbs states. (If for two Gibbs states there is a set of pure states having nonzero weight in both, then all the pure states in both decompositions must have the same value of the observable.)

(b) The conventional picture of a first-order phase transition (FOT) is that at a FOT point, two or more pure states occur and differ in the values of some O's. By Theorem 1, if two or more such pure states occurred (for flip-invariant O, if there is spin-flip symmetry), each with nonzero $\nu\kappa_J w_\Gamma$ probability, then κ_J would be nontrivial (ν–almost surely), with the different values of O segregated into distinct Gibbs states in the support of κ_J. The way this arises in the cases of O's as in example case (i), or the energy or entropy densities, is that at the FOT point, for each finite size, one or the other of the two states is favored by sample-to-sample fluctuations of disorder that couple to O locally, so in the limit, the κ_J probability of a mixture of the two is 0. One example is the random-field Ising ferromagnet, in which there is no spin-flip symmetry, and for $d > 2$ at low T, there are two pure states with opposite magnetization [35], while κ_J is nontrivial [20,36]; others are FOTs with nonzero latent heat [37], in which the local transition temperature fluctuates [38], though in those it is less clear whether both the high- and low-temperature states are present in κ_J at the FOT.

(c) We define the free energy density of a Gibbs state Γ as $\lim_{W\to\infty} F_W/W^d$ (if it exists), where $e^{\beta F_W + W^d \ln 2} = \langle e^{\beta H_W}\rangle_\Gamma$ and $H_W = -\sum_{X: X\cap\Lambda_W \neq \emptyset} J_X s_X$ [20]. The existence of the limit for short-range H_J can be proved in a similar way to that of the usual thermodynamic limit [39–44]; the invariance properties then follow easily. The proof shows directly that the free energy density is ν–almost surely a constant, independent of both J and Γ, for any Gibbs (not just any pure) state Γ, so for this observable our result is not needed. This approach extends to the magnetization and entropy densities by taking derivatives after the $W \to \infty$ limit, but the derivatives may be undefined at a FOT point, unlike in our approach above.

(d) Theorem 1, together with the L^1 ergodic theorem [45], further implies such results as that, for each X,

$$\lim_{W\to\infty}\mathbf{E}\mathbf{E}_{\kappa_J}\int dw_\Gamma(\alpha)\left|\frac{1}{W^d}\sum_{\mathbf{x}'\in\Lambda_W}(J_{\tau_{\mathbf{x}'}X}\langle s_{\tau_{\mathbf{x}'}X}\rangle_\alpha - J_{\tau_{\mathbf{x}'}X}\langle s_{\tau_{\mathbf{x}'}X}\rangle_\Gamma)\right| = 0, \tag{8}$$

even at an FOT point; these yield stronger statements of important identities [1,2] for short-range SGs.

(e) Equality of self-overlaps in the pure states in a Gibbs state is frequently used as a hypothesis—for example, in Refs. [46,47]—and that is now justified by Theorem 1. An extension of the result, under appropriate conditions, that gave equality of self-overlaps for *all* pure states in all Gibbs states in the metastate would agree with RSB [9].

(f) For technical reasons, the proof of Theorem 1 assumes that ν is n.i.p. with $\mathrm{Var} J_X > 0$ for all $X \in \mathcal{X}$ (or all even X), which excludes the EA model. Note, however, that $\mathrm{Var} J_X$, while required to be nonzero for all X (or all even X), could be taken to be arbitrarily small for all but nearest-neighbor pairs (in this example), and rapidly decaying in X. One would expect the effect of adding a very small perturbation (not changing the symmetry) to the EA model to have little physical effect; thus, the result may hold more generally. Alternatively, one can argue that there was no physical reason to assume only nearest-neighbor interactions, as multispin interactions certainly occur generically in nature, even if they are usually weak.

We now proceed to the proof of Theorem 1. The translation-invariant distribution (or measure) $\nu\kappa_J w_\Gamma$ is for triples (J, Γ, Ψ); here we use Ψ (as well as Γ) to denote an arbitrary state, and express w_Γ as $w_\Gamma(\Psi)$, such that $\int_{\Psi\in A} dw_\Gamma(\Psi) = \int_{\Gamma_\alpha \in A} dw_\Gamma(\alpha)$ for any measurable set A. In the space of pairs (J, Ψ) consisting of a bond realization and a state, we consider (Borel-measurable) invariant sets A of pairs; that is, if $(J, \Psi) \in A$, and θ is any translation or local transformation, then $(\theta J, \theta\Psi) \in A$. These sets form a sub–$\sigma$-algebra $\mathcal{I}_1$ of the σ-algebra of all Borel sets of pairs. For a set $A \in \mathcal{I}_1$, we write A_J for the set of Ψ at the specified J; then A_J changes covariantly under either a translation or a local change in J. (We will later connect these sets with the invariant observables already discussed.) For the spin-flip-invariant case, the definition of $\mathcal{I}_1$ is modified because the local transformations are restricted to $|X|$ even, and further we impose the condition that for sets A in $\mathcal{I}_1$, if $(J, \Psi) \in A$, then $(J, \bar{\Psi}) \in A$.

The formal statement we prove is the following zero-one law, which is equivalent to Theorem 1; after its proof we explain why that is so.

Proposition 1 (zero-one law).—Consider a mixed p-spin model as in the hypotheses of Theorem 1, a metastate κ_J, and sets $A \in \mathcal{I}_1$. Then, for $\nu(J)\kappa_J(\Gamma)$–almost every (J, Γ), the measure w_Γ is trivial on the sets A_J: any such set has w_Γ-measure either 0 or 1.

Proof.—First, consider the case without spin-flip symmetry. The κ_J-expectation of the measure $w_\Gamma(A_J)$ of the set A_J for given Γ is

$$\mathbf{E}_{\kappa_J} \int_{A_J} dw_\Gamma(\Psi). \tag{9}$$

By the translation covariance of κ_J, w_Γ, and A_J, this quantity is translation invariant. Hence, as the distribution $\nu(J)$ is translation ergodic, Eq. (9) must be constant—i.e., independent of J for ν–almost every J [31]. On the other hand, for any X, under a local transformation in which only J_X changes (by ΔJ_X), to first order, Eq. (9) changes by

$$\beta \Delta J_X \mathbf{E}_{\kappa_J} \int_{A_J} dw_\Gamma(\Psi)[\langle s_X \rangle_\Psi - \langle s_X \rangle_\Gamma], \tag{10}$$

using Eq. (4) and the covariance of κ_J and A_J. By the n.i.p. property, for ν–almost every given J_X, there is nonzero marginal probability for sets of $J'_X \neq J_X$ with J'_X close to J_X, so from ergodicity, Eq. (10) must be zero. Then, applying the pure-state decomposition $\Gamma = \int dw_\Gamma(\Psi)\Psi$, we have

$$\mathbf{E}_{\kappa_J} \int_{A_J} dw_\Gamma(\Psi) \langle s_X \rangle_\Psi = \mathbf{E}_{\kappa_J} \int_{A_J} dw_\Gamma(\Psi) \int dw_\Gamma(\Psi') \langle s_X \rangle_{\Psi'}. \tag{11}$$

As Eq. (11) holds for all X, it follows that the states on the two sides are equal (relabeling Ψ as Ψ' on the left):

$$\mathbf{E}_{\kappa_J} \int_{A_J} dw_\Gamma(\Psi') \Psi' = \mathbf{E}_{\kappa_J} \int_{A_J} dw_\Gamma(\Psi) \int dw_\Gamma(\Psi') \Psi'. \tag{12}$$

Both sides are weighted averages of pure states using a probability measure, so, if nonzero, they are Gibbs states up to normalization. Now, the uniqueness of the pure-state decomposition of any Gibbs state for a given J implies that there is a contradiction unless the measures on Ψ' on the two sides are the same. In particular, as A_J is independent of Γ, and on the left-hand side only a Ψ' in A_J can contribute, there is a contradiction unless on the right-hand side Ψ' almost always lies in A_J. This implies that κ_J–almost every Gibbs state Γ that has nonzero w_Γ-measure for A_J must in fact have w_Γ-measure 1 for A_J, $\int_{A_J} dw_\Gamma(\Psi) = 1$; further, this holds for ν–almost every J. Finally, for the case with spin-flip symmetry, the proof is identical except that $|X|$ is even. ■

Thus, it is impossible to "separate" pure states into complementary covariant sets A_J, A_J^c for $A \in \mathcal{I}_1$ that both have nonzero w_Γ measure. Theorem 1 follows, because an invariant observable that took different values on (disjoint Borel) sets of pure states, each with nonzero w_Γ measure, would thereby produce such a pair of sets. Conversely, for any set $A \in \mathcal{I}_1$, there is a (Borel-measurable) function on pairs (J, Ψ) that is equal to 1 on A and zero otherwise, and it is invariant, so that Theorem 1 implies Proposition 1. The observables in the examples may not all be defined for all Ψ, but it is sufficient that all are well-defined for $\nu\mathbf{E}_{\kappa_J} w_\Gamma$–almost every pair (J, Ψ). The proof of the result can be easily extended to give similar statements for more general spins and symmetries of their Hamiltonian.

To conclude, in a broad class of models we have established a property, single-replica equivalence, of nontrivial mixed Gibbs states for short-range spin systems with disorder within any fully covariant metastate construction; it asserts that, for any Gibbs state drawn from the metastate for given disorder, each macroscopic observable takes the same value in any pure state in the decomposition of that Gibbs state. As discussed above, this considerably extends older results [20,36,37] that constrain the possible structure of mixed Gibbs states in such a metastate in a disordered spin system, including at a first-order transition point. The result for self-overlaps was used as an assumption in rigorous proofs of other results [46,47]; it parallels a result [27] for the SK model [10]. The case of parts of the internal energy density leads directly to a set of identities of the stochastic stability type [1] via methods of Ref. [2]. Such identities, as well as those of Ref. [47], could play a key future role in further constraining the behavior of such systems, similar to the case of the SK model [8]. These applications illustrate the significance of this fundamental general principle, proved here.

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