On the set of pure states for some systems with non-periodic long-range order

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Abstract

We discuss the set of pure states of some models which are ordered in a non-periodic way. This includes both some results on a random model and some results based on the Thue-Morse system. We discuss the possible nature of non-periodic long-range order, and also the overlap distribution between the pure states.

1 Introduction

In this contribution we discuss some results and conceptual issues applying to either disordered models, or to "weak crystals" [14]. We will always restrict ourselves to classical lattice models. In the theory of disordered spin models, in particular in the theory of spin-glass models, there exist a number of conceptual problems, which are raised by the Parisi approach to the Sherrington-Kirkpatrick model. We shall discuss some of these and related issues, including the applicability and interpretation of these ideas for short-range models. In particular we discuss the role of boundary conditions in obtaining pure states and in describing the state structure for random models, and give an illustrative example [6].

Up to now there are various serious problems in making Parisi's theory precise. In the Sherrington-Kirkpatrick model the description in terms of an infinite number of pure states suffers from the problem that up to now one is not able to define what a pure state is. On the other hand, an ("ultrametric") distribution over pure states for short-range models cannot influence a free energy density, because the free energy density is a state-independent quantity . As the number of mathematically precise statements one can make is so rare, even a partial implementation of the theory in some caricature of the model is of interest.

We find, surprisingly, a non-trivial implementation of one the ideas of the Parisi theory, namely the existence of an overlap distribution with an ultrametric structure between the infinitely many pure states of the system, in the realm of substitution sequences. These sequences one can consider to be the pure states for toy models for systems which are ordered in a non-periodic way. This long-range order can be of the quasiperiodic type, or even less regular. We will denote such systems which break the translation symmetry of the interaction "weak crystals", cf. Aubry's [1, 2] "weakly periodic systems" or Ruelle's [40] "turbulent crystals".

2 Something about Spin-Glass models

The spin-glass models which one usually considers have Hamiltonians containing random interactions. In the case of Ising spins, for example, one takes

$$H = \Sigma_{i,j}\ J(i,j)\sigma_i\sigma_j \tag{2.1}$$

where the coupling constants $J(i,j)$ are symmetric random variables.

When for N spins the $J(i,j)$ are chosen $1/\sqrt{N} * X(i,j)$, with the $X(i,j)$ i.i.d. Gaussian random variables, we obtain the Sherrington-Kirkpatrick model [41]. In models with a spatial structure, such as for example the Edwards-Anderson models, one chooses the $J(i,j)$ from a distribution which only depends on the distance between the lattice sites i and j. In the case where the $J(i,j)$ are independent, almost nothing is known rigorously, and even at a physical level of rigour there are various controversies. One of them is about the number of "pure states" , which one should employ in the description of the presumed low temperature spin-glass phase. There are two main claims in the literature. One the one hand, based on Parisi's scheme for treating the Sherrington-Kirkpatrick (SK-) model, there is a proposal that one needs an infinite number of states [31], on the other hand there is a theory proposed by Fisher and Huse [19, 20, 21, 22], that two states should suffice in any finite-dimensional model. For some further discussion on this issue see also [5, 10, 34, 35, 36, 37]. In the Parisi description, the infinitely many pure states are arranged in a hierarchical (tree-like or "ultrametric") way. An important quantity in the theory is the overlap distribution between different states. For short-range models we will interpret the pure states as either extremal Gibbs measures, or extremal ground state measures (ground state configurations) [26, 11]. Consider two copies—replicas— of the equilibrium state μ_J^1 and μ_J^2 of the system, with the same disorder realisation.

In the Parisi theory [31] the overlap

$$q = lim_{N\to\infty}\ 1/N\ \Sigma_{i=1\ldots N}\sigma_i^1\sigma_i^2 \tag{2.2}$$

has a distribution with respect to the product measure $\mu_J^1 \otimes \mu_J^2$, called $P_J(q)$, which is non-trivial and also non-self-averaging, that is to say, for a fixed disorder realization it is concentrated on a countable number of values, while after averaging over the disorder parameter the distribution is continuous. This averaged overlap distribution occurs in the Parisi expression for the free energy density. There are various problems in implementing these ideas, both for the SK-model and in short-range interaction models. For the SK-model it is not clear how to define the (pure) states *in* the thermodynamic limit. For short-range models, on the other hand, it is known that the free energy density is a self-averaging quantity [18, 30, 42, 27], which is state-independent [17] and also not dependent on boundary conditions. Thus a quantity which is the nontrivial average of a non-self-averaging object, describing an average over different pure states, should not be expected to show up in the free energy density. Moreover there is the problem of dependence on boundary conditions. Indeed, recently Newman and Stein [37] have shown that the overlap distribution and more generally, the "canonical" mixture of the pure states, (which they call the "metastate"), when it can be defined, is self-averaging due to its translation invariance. However, their construction still allows for a non-trivial dependence on boundary conditions. The solution of the existence question is non-trivial, due to the fact that the obvious approach (take say free or plus boundary conditions in finite volumes, and take the infinite volume limit) may not lead to a well-defined thermodynamic limit, a phenomenon described as "chaotic size dependence" [35]. Here we want to illustrate some of these boundary condition problems on a model with random site disorder, the randomly gauge transformed Potts model [6]. The first issue which we will consider is the question of *weak* versus *strong* uniqueness of the Gibbs measure for random models. If for each pair of disorder-independently chosen sequences of boundary conditions one approaches the same infinite-volume pure state (which is still disorder-dependent), for almost every realization of the disorder, we say that *weak* uniqueness applies. *Strong* uniqueness means that there is only one pure state for almost every realization of the disorder. If there are other pure states, which are only obtainable via disorder-dependent boundary conditions, this means that the uniqueness is not strong [7, 33, 44]. One example where this phenomenon is known to happen is the Ising spin-glass on the Bethe lattice, at temperatures between the spin-glass and the ferromagnetic critical temperatures [8, 3]; another example is the high temperature regime of extremely-long-range interactions [23, 24]. Here we give an example with a nearest neighbour interaction on a regular lattice Z^d, $d \geq 2$. The Hamiltonian we will consider is

$$H = \Sigma_{i,j} - \delta(\xi_i \sigma_i, \xi_j \sigma_j) \tag{2.3}$$

where the Potts spins $\sigma_i = 1...q$, and the ξ_i are random permutations of the q Potts spins, chosen independently at each site of the lattice. This model is equivalent to a Potts ferromagnet, after applying a random gauge transformation. The pertinent observation we make here is that any fixed boundary condition, after undoing the random gauge transformation, becomes random. At the transition temperature, for large q, a disordered pure state (extremal Gibbs measure) coexists with q ordered pure states. Choosing the spins at the boundary randomly, favours the disordered state (in which neighbouring spins typically are different) over the q ordered ones. This statement can in fact be made rigorous. This implies for the Hamiltonian defined above that weak uniqueness holds, but not strong uniqueness, *at* the transition temperature [6]. Another simple observation about this model is that while for periodic boundary conditions in the thermodynamic limit one obtains the equiweighted mixture of the $q+1$ pure states [4], for antiperiodic or fixed translation invariant boundary conditions (say $\sigma = 1$ for each boundary spin) we obtain the pure disordered state. Thus, even though the mixture is (trivially) translation invariant and self-averaging, it is still dependent on boundary conditions.

The maximum minus the minimum value of the overlap, taken over all pairs of pure states, defines the Edwards-Anderson order parameter [12]. This definition in the terms introduced above is a *strong* definition, the example above illustrates that the weak and the strong version of this order parameter do not necessarily coincide, a question which was left open in [12].

3 Some Results about Weak Crystals

In this section we will discuss a number of issues which we will illustrate on the (Prouhet-)Thue-Morse substitution system[29]. We consider the sequences generated by the substitution rule $+ \rightarrow +-$ and $- \rightarrow -+$, hence the sequence $+-\ -+\ -++-\ -++-+--+\ -++-+--++--+-++-\ldots$, its translates and limits (the orbit closure) are the sequences we will consider. They support exactly one translation-invariant probability measure μ_{TM} (this property is called "unique ergodicity of the measure") and they form a minimal translation invariant set, that is, they give rise to a strictly ergodic [43] system. A set is minimal if it is closed, translation-invariant and non-empty, and has no proper subset with this property. Physically this means that the set does not contain configurations with defects. We will say that μ_{TM} has long-range order because at large distances correlations do not factorize:

$$lim_{n\to\infty}\mu_{TM}(\sigma_0\sigma_n) \neq \mu_{TM}(\sigma_0)^2 = 0 \tag{3.1}$$

This can be seen easily because of the fact that the correlations are scale-invariant in the sense that

$$\mu_{TM}(\sigma_0\sigma_n) = \mu_{TM}(\sigma_0\sigma_{n*2^p}) \tag{3.2}$$

for all n and p. In general these correlations are non-zero. The long-range order is non-periodic, in the sense that one cannot write μ_{TM} as an average (mixture) of periodic pure states. Each measure in which the translation symmetry of the interaction is broken in the sense that it is not a mixture of pure translation invariant states and moreover has some positional long-range order in the sense that some correlation functions do not factorize at large distances, we will call a "(weak) crystal" [14].

(It is possible to have uniquely ergodic measures which have very good mixing properties, but are not pure states. Therefore the notions of long-range order in the sense of having long-range correlations and in the sense of being a mixture of pure states are not necessarily equivalent. Such "unique disordered" measures which also can be unique translation invariant ground states have been discussed in [39].)

The measure μ_{TM} is the *only* translation invariant ground state measure of some fast-decaying 4-spin interaction $V(i,j,k,l)$ with Hamiltonian

$$H = \Sigma V(i,j,k,l)(\sigma_i+\sigma_j)^2(\sigma_k+\sigma_l)^2 \tag{3.3}$$

As an aside, we remark that both the properties of being a strictly ergodic system and having non-perodic long-range order are typical for ground states of summable interactions [1, 38, 39, 32].

The construction of these interactions is based on the observation [25] that pairs of equal neighboring spins occur only at even distances from each other in any Thue-Morse sequence, combined with scale invariance. What then is needed to complete the argument is to show that the above property actually fully characterizes the

Thue-Morse system. As for positive temperatures, it can be shown that a similar non-periodic long-range order occurs, but for slowly decaying 4-body interactions [15]. This slow decay is unavoidable in a one-dimensional model, it is hoped that in three or more dimensions a fast decaying interaction will lead to the same result [16]. Another way of studying non-periodic long-range order is to concentrate on the spectral properties of the Thue-Morse system. In the physics literature it is often claimed that there occurs purely singular spectrum, see for example [9], although mathematically the description of the Thue-Morse system, considered as a dynamical system in the sense of ergodic theory, gives rise to a mixed discrete/singular spectrum. The explanation in physics terms of this apparent contradiction is in that if one considers the Thue-Morse system as a lattice gas model there is a distinction between the atomic spectrum which is singular and the molecular spectrum which can be discrete. To be precise, the Fourier transform of $\mu_{TM}(\sigma_0\sigma_n)$ is a singular continuous measure (the atomic diffraction spectrum or structure factor), while the Fourier transform of $\mu(X_0X_n)$ is countable discrete (the molecular diffraction spectrum), if for example $X_i = \sigma_0\sigma_{i+1}$. Thus the "molecule" consists of 2 equal neighbouring atoms.

As remarked before, the Thue-Morse sequences are pure ground states for some translation-invariant interaction. The translation-invariant measure on them is the "canonical" mixture (in the language of [37] the metastate). It is hence possible to study the overlap distribution with respect to this measure between the different pure states [13]. The first result is for the Thue-Morse overlap distribution:

$$lim_{N\to\infty}(1/N\ \Sigma_i\sigma_i^1\sigma_i^2) = 0 \tag{3.4}$$

almost surely with respect to the product measure $\mu_{TM}\otimes\mu_{TM}$.

The fact that the overlap distribution is trivial follows from a well-known argument in ergodic theory, which needs a slight modification in our case. The original result (see for example Walters [43]) shows that if for a measure μ the translation operator has no point spectrum, that is, the measure is weak mixing, the product measure $\mu\otimes\mu$ is ergodic, and hence the overlap distribution, because it is translation invariant, is a constant. As a side remark we note that the property of weak mixing is in fact compatible with the existence of long-range order, the absence of long-range order is a strictly stronger mixing property. The Thue-Morse system behaves like a weakly mixing system on observables which are odd under a global spin-flip [29]. The second result is for the "molecular" overlap distribution of the "molecules" $X_i = \sigma_i\sigma_{i+1}$. These molecules form a so-called Toeplitz system [28]. A Toeplitz sequence can be constructed by first taking half of the lattice sites (with probability 1/2 the sites with even coordinates, with probability 1/2 the sites with odd coordinates) and occupying them with -1. ¿From the as yet unoccupied sublattice we occupy one of the two period-four sublattices with pluses; again, which one of the two sublattices becomes occupied, is chosen randomly. We repeat this procedure, putting in pluses and minuses alternatingly at each step. The Toeplitz system is known to be almost periodic in the sense that the translation operator has pure point spectrum, with infinitely many generators [28]. The overlap distribution is concentrated on a countable number of values, and the pure states (the Toeplitz sequences) are organized in an ultrametric way. The overlap between two sequences depends only on which is the first step at which the choice of the sublattice to be occupied is different. This result is fully consistent with the observation of Newman and Stein [37] that the (non-)triviality of the overlap distribution has nothing to do with non-self-averaging; indeed, because there is no randomness here, self-averaging is trivially satisfied, but the self-averaging overlap distribution is non-trivial, and in fact even ultrametric. As a side remark we mention that also for the Fibonacci system (which is quasiperiodic) the overlap distribution can be computed, and that it has a continuous part [13].

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