On the prevalence of non-Gibbsian states in mathematical physics

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Abstract

Gibbs measures are the main object of study in equilibrium statistical mechanics, and are used in many other contexts, including dynamical systems and ergodic theory, and spatial statistics. However, in a large number of natural instances one encounters measures that are not of Gibbsian form. We present here a number of examples of such non-Gibbsian measures, and discuss some of the underlying mathematical and physical issues to which they gave rise.

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1 Introduction

1.1 Gibbs measures according to DLR

Gibbs (or DLR) measures, or Gibbs states, are the main objects in classical equilibrium statistical mechanics. They were introduced in the sixties by Dobrushin, Lanford and Ruelle, as probability measures on systems of infinitely many particles (or spins) in infinite volume, satisfying a set of consistent conditional probabilities for configurations in finite volumes, conditioned on external configurations. This is expressed by the so-called DLR equations. These conditional probabilities are of the Gibbsian form \( \text{Cst} \exp -\beta H \), where the Hamiltonian \( H \) describes the interactions between particles both inside the volume and between the volume and the outside. In particular for classical lattice models, the theory of infinite-volume statistical mechanics has developed in substantial detail, see e.g. [18]. Gibbs measures also play a role in various other domains, such as Dynamical Systems, non-equilibrium theory, Interacting Particle Systems, Euclidean Quantum Field Theory, ergodic theory, spatial statistics and pattern recognition.

For finite-range interactions, Gibbs measures satisfy a spatial Markov property, for regular infinite-range potentials a weak form thereof, which goes by the names of the “almost Markov” or “quasilocality” property. For discrete bounded-spin models this property is equivalent with the conditional probabilities being continuous functions of the boundary conditions, in the product topology.

It is a nontrivial result that in fact equivalence holds: any measure whose conditional probabilities are quasilocal is a Gibbs measure for a regular interaction, once it satisfies a natural nonnullness condition.

1.2 Effective descriptions and the Gibbs-non-Gibbs question

In many parts of statistical physics use is made of effective interparticle Hamiltonians. That is, one tries to describe a system in which one forgets about small-scale details, but that still can be described by a Hamiltonian, which contains only properties of larger-scale entities. (E.g. an effective molecular Hamiltonian does not include properties of the constituent atoms, electrons or quarks, but only -effective- forces between molecules). To make this notion mathematically precise, that is, to decide if such an effective Hamiltonian exists, the quasilocality property mentioned above needs to be checked for an appropriate measure (in the example above, that would be the measure restricted to all the molecular degrees of freedom). However, it has turned out, initially rather surprisingly, that in many natural examples this quasilocality property is violated, and no regular interaction can be found: the measure is non-Gibbsian. Often, the Gibbsian or non-Gibbsian character of a measure depends on certain parameters of the problem under consideration, such as temperature, magnetic field, time, or rescaling parameters, in an a priori non-obvious way.
Examples of such contexts that occur in statistical mechanics are Renormalisation Group theory, the theory of disordered systems and the theory of stochastic dynamics (Interacting Particle Systems).

In Renormalisation Group theory, a Renormalisation Group map is a kind of coarse-graining map. One considers only a subset of coarse-grained or “renormalised” objects (spins, fields), and then considers the restriction or projection of Gibbs states on those. In physical terms, one integrates out some short-range degrees of freedom. In probabilistic terms, one takes the marginal of a probability measure on a subset of random variables, often called the set of “block spins”. This renormalised measure then is supposed to be describable by a renormalised Hamiltonian. The philosophy of Renormalisation Group theory is based on studying the properties of this map from original to renormalised Hamiltonians in some appropriate space. The ultimate goal is to determine the fixed points of this map, together with their stability properties, and to relate them to the critical behaviour inside corresponding “universality classes”, which are classes of physical systems with the same critical exponents. In this way, critical behaviour is expected to follow from the properties of certain Renormalisation Group maps. This paradigm is based on the assumption that such a map exists, in other words, that the renormalised measure is in fact a Gibbs measure.

It is precisely this step which has turned out to be doubtful in a variety of circumstances. The first clear indication that defining a well-behaved Renormalisation Group map might be problematical was found by Griffiths and Pearce [19] and the nature of the problem was identified shortly after by Israel [20]. A first extensive analysis appeared in [6]. We will see the mechanism in the particularly simple example of the decimation transformation later on. Although in a majority of cases the predictions of the Renormalisation Group approach about the nature of phase transitions and critical properties are not affected, in some cases, especially in the theory of first-order transitions, non-Gibbsianness results restricted and even excluded Renormalisation Group descriptions proposed in the physics literature.

Follow-up studies identified a variety of other occurrences of non-Gibbsian measures. A direct generalisation of the above treatment of block-spin maps often works in considering single-site renormalisations, including dicretisations, the so-called “fuzzy” or “amalgamation” maps [2, 9, 34].

Another example is provided by low-temperature Gibbs measures, subjected to a high-temperature or infinite-temperature Glauber (stochastic spin-flip) dynamics. This is an example from the area of interacting particle systems [28], which models a fast heating procedure. The initial Gibbs measure after some finite time can become non-Gibbsian. So instead of raising the temperature [31], one may altogether lose the notion of effective temperature [7]. The proofs of such non-Gibbsianness results are quite similar to the ones in a Renormalisation Group context, but with the distinction that one may consider now the marginal of a two-time (initial time and end time) system which is of a Gibbsian form. One can in fact go into more detail, and perform a path-space analysis in which the whole dynamics is included [8].
Yet another family of occurrences of non-Gibbsian measures is in the theory of disordered spin systems [1]. In such systems the Hamiltonians contains, next to the spin variables, disorder variables, e.g. occupation numbers or random fields. When a “quenched” disordered measure is non-Gibbsian, that means that one cannot write it as an “annealed” measure, that is a Gibbs measure for an effective Hamiltonian. Physically, in a quenched, fast cooled, system the disorder is frozen, while the spins equilibrate; in other words, the disorder variables are slow and the spins fast. In annealed, slowly cooled, systems the disorder variables equilibrate with the spins, and there is only one timescale, and there are no fast or slow variables. Probabilistically, for a quenched measure the disorder variables are independent, identically distributed; conditioned on the disorder variables the spins are distributed according to a Gibbs measure. Annealed measures are Gibbs measures on a product space of spin and disorder variables. The impossibility to write a quenched measure as an annealed measure is in contrast to what has been proposed in the physics literature as the Morita approach [11, 23, 25] where one aims to compute a “grand potential”, an effective interaction for a quenched measure, viewed as a Gibbs measure (an annealed one).

2 Gibbs measures and non-Gibbsian measures

2.1 Notation and Definitions

We will consider lattice spin systems with a single-spin space $\Omega_0$, on a lattice $\mathbb{Z}^d$, and a configuration space $\Omega = \Omega_0^{\mathbb{Z}^d}$. We will, for simplicity, mainly consider Ising models, for which $\Omega_0 = \{-1, +1\}$. We will indicate the spin variables at site $i$ by $\sigma_i$, $\omega_i$, $\eta_i$, and similarly spin configurations in a volume $\Lambda$ by $\sigma_\Lambda$, $\omega_\Lambda$, $\eta_\Lambda$.

We will consider Gibbs measures, which are defined for absolutely summable interactions $\Phi$ via the DLR equations. An interaction $\Phi$ is a (translation-invariant) collection of functions $\Phi_X(\sigma_X)$. Each $\Phi_X$ describes an energy contribution in a finite subset $X$ of the lattice. Absolute summability means that $\sum_{\theta \in X} \|\Phi_X\| < \infty$. This implies that any finite change in an infinite-volume configuration only comes with a finite energy cost (or gain), uniformly in the external configuration. Such interactions form an interaction (Banach) space. The DLR equations say that given an external configuration $\eta_\Lambda^e$, the probability (density) of configurations in a volume $\Lambda$ is given by the Gibbs expression

$$
\mu_\Lambda^{\eta_\Lambda^e}(\sigma_\Lambda) = \frac{\exp(-\beta H^\Phi_\Lambda(\sigma_\Lambda, \eta_\Lambda^e))}{Z^{\eta_\Lambda^e}_\Lambda}.
$$

where

$$
H^\Phi_\Lambda = \sum_{A: A \cap \Lambda \neq \emptyset} \Phi_A(\sigma_\Lambda, \eta_\Lambda^e)
$$

This should hold for all volumes $\Lambda$, internal configurations $\sigma_\Lambda$ and external configurations $\eta_\Lambda^e$. The conditional probabilities given above have a continuous (in the product topology) version due to the summability of the interaction. This means
that the conditional expectation of any local observable cannot change much between two configurations which are identical in a sufficiently large environment, and are different only far away, whatever the configuration in this finite environment is. Each such configuration is thus a point of continuity for each conditional expectation.

It also turns out to be true that a measure having a continuous version of its conditional probabilities, and satisfying a nonnullness (or “finite-energy”) condition, is a Gibbs measure for a reasonable interaction. The finite-energy condition for Gibbs measures follows immediately from the absolute summability. See e.g. [6, 15, 18] for further background.

In the standard nearest-neighbour Ising model we have

\[-H_\Lambda = \sum_{<i,j> \in \Lambda} \sigma_i \sigma_j + \sum_{<i \in \Lambda, j \in \Lambda^c>} \sigma_i \eta_j.\]

2.2 Decimating the Ising model, a paradigmatic example

Decimation, in which one considers just a subset of the spins, is a conceptually easy example of a Renormalisation Group map. Let us consider the even decimation of the two-dimensional Ising model, in which \(\sigma'_{i,j} = \sigma_{2i,2j}\). Thus we consider only a quarter of the spins, namely those on sites with both coordinates even. Those primed spins will be our renormalised or “visible” spins. If the original Gibbs measure is at low enough temperature, the primed measure defined by taking the marginal of this measure on the primed spins is non-Gibbsian. Indeed, let us fix all primed spins in a large box in an alternating configuration. Then the other, “invisible” spins in the box don’t feel any influence from them, due to cancellation effects. Thus the conditioned system of the invisible spins, forms a spin system on a lattice with periodic holes, a “decorated” lattice.

Any configuration of the visible (renormalised) spins acts as a condition in a conditional probability of the invisible-spin system, conditioned on it. But it is the alternating configuration which will be the one that we will show to be responsible for non-Gibbsian behaviour.

If in an annulus outside the box all visible spins are plus (that is, they are pointing upwards), we have a plus-like boundary condition, for any condition of the invisible spins outside the annulus. Now let us unfix the visible spin at the origin. Then this spin has a positive expectation, larger than some constant, uniformly in the size of the box. Making the visible spins minus outside the box produces a minus expectation. Thus the visible spin at the origin, conditioned on a large surrounding alternating configuration of visible spins has a large change in expectation, when one changes the configuration far away.

Notice that the phase transition in the system of invisible spins gets translated in a nonlocal influence –action at a distance– between the visible spins, violating the quasilocality condition for the measure on the visible spins. This renormalised measure thus is non-Gibbsian. The alternating configuration is a point of discontinuity of the spin at the origin, conditioned on (considered as a function of) the
visible spins. This argument works if the temperature is low enough, as the dec-
orated lattice has a strictly lower transition temperature than the original Ising
model.

Although there are other choices possible than the alternating configuration,
we expect that in fact for most choices of the primed-spin configuration continuity
holds.

It can be shown that renormalising different Gibbs measures for the same
interaction results in the renormalised measures being all Gibbsian or all non-
Gibbsian.

By similar arguments other decimated measures become non-Gibbsian. This
includes a finite number of decimations applied to Ising models in dimension
at least two in a weak field at low temperatures, or (arbitrarily often) repeated
decimations in zero field at low temperatures. In the zero-field case the alternating
configuration is neutral, in that it does not favour either the plus or the minus
phase. The Ising model with a small plus field, does not exhibit multiple phases,
but conditioning on a configuration which is predominantly minus can induce a
phase transition. Thus the presence of a phase transition in the original system is
neither necessary, nor sufficient, for the transformed measure to be non-Gibbsian.

On the other hand, at high temperatures, and also for decimation in strong
fields, the transformed measures are Gibbsian. Thus, as Griffiths and Pearce
\[19\] already noticed, one can define Renormalisation Group maps where one does
not really need it, away from phase transitions (and even then not always). For
mathematical details, see \[6\]. But even then, the Renormalisation Group map on
the space of summable interactions has unexpected spectral properties, indicating
that this space, although giving rise to proper Gibbs measures, is already too large
to properly implement Renormalisation Group ideas in (see \[35\]).

2.3 Extensions I: Renormalisation, stochastic dynamics,
discretisations

The occurrence of non-Gibbsian measures is actually quite widespread. Indeed, in
a topological sense, they occur generically, for a residual set (that is, a countable
intersection of dense open sets) in the set of probability measures \[21\].

Similar results as proven above for decimation can be proven for a vari-
ety of Renormalisation Group transformations. For example, one can prove
non-Gibbsianess for Ising models subjected to majority-rule transformations (in
which a renormalised spin equals the sign of the majority of the spins in a block)
at low temperatures in any external field, various random versions thereof (the
Kadanoff transformations), etc.

Beyond Renormalisation Group transformations, similar results hold also for
evolved Ising systems, under a high-temperature Glauber (stochastic spin-flip)
dynamics. Starting from a low-temperature Gibbs measure in the phase-transition
regime, for a short time the evolved measure is Gibbsian, but at larger times it
becomes non-Gibbsian, and then it stays so for any finite time in this transient,
nonstationary, regime. This is true although the measure converges exponentially fast to a very well-behaved high-temperature Gibbs measure. Other sources of non-Gibbsian measures are single-site coarse-grainings. In the dynamical case the visible spins are evolved spins, and the invisible ones the initial spins. For single-site coarse-graining (fuzzy [34] or amalgamation [2]) maps, fine details become invisible, and one can only observe coarser details, the fuzzy, or amalgamated, spins.

In all these examples, the presence of a transition in the invisible spins, conditioned on some special configuration of the visible spins, gets translated into the fact that this special configuration is a point of discontinuity (a “bad point”). If for no possible conditioning a phase transition occurs, the transformed or evolved measure is a Gibbs measure. This typically happens if the transformation is close to unity. Examples of Gibbsian regimes are very-short-time evolutions, or very fine discretisations for initial systems that are at not too low temperatures.

Let me emphasize that the absence or presence of these transitions is for conditioned systems, and not for the original, untransformed system, which may or may not be in a phase transition regime.

2.4 Extensions II: Trees and Mean-Field theory. Path approach

Related results can be proven in a mean-field setting, in this case, the (dis)continuity to be investigated of, for example, a spin expectation, is not any more of that of a function of the external configurations in the product topology. Rather, the conditional expectation value of a spin is seen as a function of some order parameter, such as a magnetisation. This approach has especially been pioneered by C. Külske, see e.g. [26, 30].

In the above context, the “bad points” are exceptional, that is they have measure zero. In other situations, in particular in the Random Field Ising model, and also for evolved unstable Gibbs measures on trees, it can even happen that almost all or all configurations become bad [5, 24]. Gibbs measures on trees differ from those on lattices in that, due to the large boundary terms, at low temperatures one can have metastable and even unstable homogeneous Gibbs measures, corresponding to different types of solutions of a self-consistency equation. In this sense they violate the variational principle that says that all Gibbs measures minimise a free energy density. Due to this, the Gibbsian and non-Gibbsian properties of the evolved measures can be very different for different initial Gibbs measures for the same initial interaction.

Recently, in the dynamical Gibbs-non-Gibbs transitions a more refined analysis has led to the identification of bad objects (bad points or bad measures) as points or measures which can have different, competing, histories. A large-deviation analysis on the level of trajectories in a space of paths then becomes required. The corresponding rate functions are sums of an initial rate function, and a dynamical rate function, which can be computed as a particular Lagrangian by the methods developed in [14]. For these developments we refer to [8, 13, 33, 17]. A bad value
of the magnetisation then would be one which can have two quite different origins, starting from either a positive or a negative value, for example.

2.5 Further generalizations. Other sources of non-Gibbsianness.

The above description has been mostly about discrete-spin models, but extensions to continuous, possibly unbounded, spin systems also exist. In the bounded-spin case of vector models, the case which has in particular been studied is that of stochastic time evolutions, see e.g. \[10\]. Continuous-spin systems have been studied either be subjected to single-site or weakly interacting diffusions, or (as mentioned before) to discretisation. In the unbounded-spin case, the notion of what is a Gibbs measure for a “decent” interaction becomes a bit more arbitrary. For some of the literature on this issue, see \[3, 27, 32\]. In the case of discretisation of vector spins one determines the angle of an XY (vector) spin up to finite precision, obtaining a “visible” clock-spin measure, which in the Gibbsian situation has a summable clock-spin interaction, but at very low temperatures becomes non-Gibbsian \[9\].

Other examples of non-Gibbsian measures abound, including random-cluster (Fortuin-Kasteleyn) measures, invariant measures for stochastic evolutions, g-measures, which satisfy a one-sided version of the continuity (Gibbs) property of their conditional probabilities, lower-dimensional projections of Gibbs measures, sign-fields of massless Gaussians,... See e.g. \[16\] and for earlier results \[15, 6\] or the special Vol 10(3) of the journal “Markov Processes and Related Fields”. Next to a violation of the quasilocality property, another way of proving non-Gibbsianness which works in some of the above cases, is showing either anomalous large-deviation properties, or a violation of the non-nullness (or finite-energy) condition.

Another, as yet unexplored, direction is about quantum statistical mechanical systems. In this case one is still looking for a characterisation of Gibbs or KMS states which can actually be checked in examples. Conditional probabilities have no analogue in a quantum context, which makes the above classical analysis not applicable.

3 Conclusions

Although a variety of examples of non-Gibbsian measures have by now been discovered, the significance of this fact still appears somewhat controversial.

Mathematically, the phenomenon seems quite widespread, and we have developed a fairly systematic approach to handle a lot of examples, many of which are measures showing up in natural circumstances.

One response has been to try to make non-Gibbsian measures “as Gibbsian as possible”, by weakening the definition of what a Gibbs measure is. This approach, which was suggested by R.L. Dobrushin, has led to the notions of almost, weak and intuitively weak Gibbs measures \[29, 4, 12\]. As a warning, it should be noted
that the quenched Random Field Ising measure, which can be shown to be weakly
Gibbsian, (that is, one can define a Hamiltonian which is defined almost every-
where with respect to this measure), violates the variational principle [24]. This
implies that measures from these classes can be substantially less well-behaved
than regular Gibbs measures.

Physically, non-Gibbsianness reflects the presence of some nonlocal correla-
tions, describable by interactions that have an extremely long range. They are
not even summable and represent some “actions at a distance”. In the theory of
the Renormalisation Group, as applied to critical phenomena, the appearance of
long-range interactions often leads to these interactions belonging to a different
universality class, even if they are summable. Hence there is serious cause for
concern if terms appear which are even worse. Ideally, a Renormalisation Group
map would act on a subspace of interactions within the same universality class.

The fact that a proposed algorithm is mathematically ill-defined may or may
not invalidate results which are obtained by approximate methods. However, for a
mathematical physicist to develop a systematic understanding when and when not
to trust renormalisation-group folklore remains a big challenge. Similar questions
arise if one tries to introduce effective temperatures, or effective potentials of the
Morita (quenched-as-annealed) type.

If one can prove the Gibbsianness of a measure, one can in principle trust
numerical approximations, and hopefully obtain some proper error bounds. How-
ever, even that appears to be a much harder problem than one would a priori expect [22].

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