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REGULARITY PROPERTIES AND PATHOLOGIES OF POSITION-SPACE RENORMALIZATION-GROUP TRANSFORMATIONS

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We reconsider the conceptual foundations of the renormalization-group (RG) formalism. We show that the RG map, defined on a suitable space of interactions, is always single-valued and Lipschitz continuous on its domain of definition. This rules out a recently proposed scenario for the RG description of first-order phase transitions. On the other hand, we prove in several cases that near a first-order phase transition the renormalized measure is not a Gibbs measure for any reasonable interaction. It follows that the conventional RG description of first-order transitions is not universally valid.

1. INTRODUCTION

A principal tenet of the renormalization-group (RG) theory of phase transitions [1] is that the RG map, defined on a suitable space of Hamiltonians, is *smooth* (i.e. analytic or at least several-times differentiable), even on phase-transition surfaces. The singularities associated with critical points [1] and first-order phase transitions [2] are then explained in terms of the behavior of the RG map under infinite iteration.

This picture of a smooth RG map has, however, been questioned, particularly as regards the behavior near a *first-order* phase transition. On the one hand, several groups [3,4,5,6] have reported numerical evidence suggesting that the RG map is *discontinuous* on the first-order transition surface. On the other hand, Griffiths and Pearce [7] have pointed out some "peculiarities" of the commonly used discrete-spin RG transformations (decimation, majority rule, etc.) in the low-temperature regime[‡]; and Israel [9] showed that in at least one such case the expectations of renormalized observables exhibit characteristics incompatible with a Boltzmann prescription, i.e. the renormalized measure is *non*-

[†]Speaker at the conference.

[‡]Similar peculiarities, and also different ones, are reported in [8].

Gibbsian.

We have reconsidered the conceptual foundations of the RG formalism [10], and have proven that of these proposed pathologies, the only type that can (and does) occur is the Griffiths-Pearceisrael type. We prove that the RG map, defined on a suitable space of interactions (= formal Hamiltonians), is always single-valued and Lipschitz continuous on its domain of definition. On the other hand, we prove, extending Israel's [9] argument, that in several cases the RG map is ill-defined for a much more basic reason: the renormalized interaction may fail to exist altogether. Moreover, this pathology can occur in the vicinity of - not only at — a first-order phase transition: for the Ising model in dimension $d \geq 3$ it occurs in an open region $\{\beta > \beta_0, |h| < \epsilon(\beta)\}$.

Our point of view is the following: An RG map is defined initially as a rule (deterministic or stochastic) for generating a configuration ω' of "block spins" given a configuration ω of "original spins". Mathematically this is given by a probability kernel $T(\omega \rightarrow \omega')$. One can then define a probability distribution $\mu'(\omega')$ of block spins from any given probability distribution $\mu(\omega)$ of original spins:

$$\mu'(\omega') \equiv \sum_{\omega} \mu(\omega) T(\omega \to \omega') . \tag{1}$$

In other words, the RG map is easily defined as

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a map from measures to measures. On the other hand, most applications of the renormalization group assume (and need) that the RG map is defined as a map from Hamiltonians to Hamiltoniums. That is, μ is chosen as the Gibbs measure for a statistical-mechanical system with Hamiltomian H, and μ' is assumed to be the Gibbs measure for a system with some Hamiltonian H'. This is taken to define an RG map R on some suitable space of Hamiltonians, by the diagram

$$\begin{array}{cccc} \mu & \xrightarrow{\mathbf{T}} & \mu' \\ 1 & & \downarrow \\ \mathbf{H} & \xrightarrow{\mathbf{R}} & \mathbf{H}' \end{array}$$
 (2)

Formally the relation between a Hamiltonian and its corresponding Gibbs measure is given by $\mu =$ const $\times e^{-B}$, and hence the RG map on the space of Hamiltonians is defined *formally* by

$$H'(\omega') = -\log\left[\sum_{\omega} e^{-H(\omega)} T(\omega \to \omega')\right] + \text{const}.$$
(3)

However, this formula is valid only in finite volume; in infinite volume, the Hamiltonian $H(\omega)$ is ill-defined (its value is almost surely $\pm \infty$), and the connection between a formal Hamiltonian (more precisely, an interaction) and its corresponding Gibbs measure(s) is much more complicated [11]. We emphasize that this is not a mere mathematical nicety: it contains the fundamental *physics* of phase transitions, which occur only in infinite volume.

Let us give a concrete example. Consider the Ising model in dimension $d \ge 2$ at low temperature $(\beta \gg \beta_c)$ and zero-magnetic field. At such a point there are two pure phases (= extremal translation-invariant infinite-volume Gibbs measures), μ_+ and μ_- . These phases are characterized by a large magnetization $\pm M_0$ and a small correlation length ξ . After a block-spin transformation T, such as majority-rule, the image measures μ'_{\pm} will have a yet larger magnetization $\pm M'_0$ and a yet smaller correlation length ξ' . We now ask: These image measures μ'_{\pm} are typical of what kind of Hamiltonian?

The conventional scenario [2] is that the RG flow is toward lower temperatures along the h = 0

 $line^{3}$; in this case the two image measures μ'_{\pm} would be Gibbsian for the same Hamiltonian H'. A different possibility was suggested by Decker, Hasenfratz and Hasenfratz [5], in which Hamiltonians H with an infinitesimal positive (resp. negative) magnetic field h would get mapped by a single RG step to renormalized Hamiltonians H' having a strictly positive (resp. strictly negative) magnetic field h'. Furthermore, at h = 0 the image measures μ'_{\pm} would be Gibbsian for different Hamiltonians H_{\perp}^{i} having (among other couplings) magnetic fields of different sign. In this scenario, the RG map R would be discontinuous as one approaches the phase-transition line, and multi-valued on that line. 4 Both scenarios are consistent with the intuitive idea that magnetization increases and correlation length decreases under the RG map.

We have proven [10] that the second scenario exampt occur: the RG map \mathcal{R} is always singlevalued and Lipschitz continuous wherever it is defined. On the other hand, in at least some cases [9,10] the first scenario is not sulid either, because the Hamiltonian H' fuils to exist at all. That is, it can occur that the image measure p' is not a Gibbs measure for any reasonable Hamiltonian.

2. GENERAL FRAMEWORK

Our results apply to systems on a lattice $\mathcal{L} = \mathcal{L}^d$ characterized by a single-spin space Ω_0 , which comes equipped with a physically natural singlespin measure μ^0 . The infinite-volume configuration space Ω is the Cartesian product $(\Omega_0)^{\mathcal{L}} = \{\omega = (\omega_x)_{x \in \mathcal{L}} \mid \omega_x \in \Omega_0\}$. We consider "renormalization maps" T from an original (or object) system $(\Omega = \Omega_0^{\mathcal{L}}, \mu^0)$ to an image (or renormalized) system $(\Omega' = \Omega_0^{\mathcal{L}}, \mu^0)'$ such that: (T1) T is a probability kernel; (T2) T carries translation-invariant measures on Ω into translation-invariant measures

[§]More precisely, the flow would take place in an infinite-dimensional space of couplings, but would respect the $\sigma \rightarrow -\sigma$ symmetry; *no* magnetic fields, three-spin couplings or other *odd* interactions would arise.

[¶]This possibility was suggested earlier, in the context of the 3-state Potts model in three dimensions, by Blöte and Swendsen [3] and with especial clarity by Rebbi and Swendsen [12, p. 4099].

on Ω' ; and (T3) *T* is strictly local in position space, that is, there exists a number $K < \infty$ (volume compression factor) such that the image spins in each region Λ' depend only on the original spins in a certain region Λ with $|\Lambda| \leq K |\Lambda'|$. This set-up includes all of the usual deterministic or stochastic real-space renormalization schemes: decimation, majority rule and Kadanoff transformations. It excludes, due to the strict locality requirement, most momentum-space renormalization maps (but we conjecture that our results extend also to such maps).

The map $\mu \mapsto \mu'$ induced by T is always welldefined; the problems arise when trying to complete (2) to define the renormalization-group map \mathcal{R} on Hamiltonians. We consider only a *single* application of the RG map, so the semigroup property of the "renormalization (semi)group" plays no role for us.

Let us introduce some needed notions of infinite-volume statistical mechanics [13,14]. To make rigorous the idea of "formal Hamiltonian" (collection of one-body terms, two-body terms, etc.), we define an *interaction* to be a family $\Phi = (\Phi_A)$ of functions Φ_A : $\Omega \to \mathbf{R}$, such that for each finite $A \subset \mathcal{L}$, the function Φ_A depends only on the spins in the subset A. The interactions are assumed to be *translation-invariant*. As in a renormalization procedure interactions proliferate, we must allow interactions among arbitrarily many spins simultaneously, and therefore we must impose certain summability conditions: We consider the (Banach) space \mathcal{B}^1 of translation-invariant continuous interactions with norm

$$\|\Phi\|_{\mathcal{B}^{1}} \equiv \sum_{A \ni 0} \|\Phi_{A}\|_{\infty} < \infty , \qquad (4)$$

where $\|\Phi_A\|_{\infty} = \sup_{\omega} |\Phi_A(\omega)|$. Condition (4) ensures that for each *finite* volume Λ and boundary condition τ , there is a well-defined Hamiltonian $H_{\Lambda,\tau}^{\Phi}$ and Boltzmann-Gibbs distribution $\pi_{\Lambda,\tau}^{\Phi}$. The *infinite-volume* Gibbs measures for interaction Φ are then defined [11] to be those measures whose conditional probabilities on finite volumes are exactly the measures $\pi_{\Lambda,\tau}^{\Phi}$.

Some remarks are in order. First, we notice that the requirement (4) makes our results applicable,

for practical purposes, only to systems of bounded spins. Second, the same Hamiltonian (or, more precisely, the same conditional probabilities) can be expressed via different interactions. We should not distinguish between such interactions, which are therefore called *physically equivalent*. With this identification Griffiths and Ruelle [15] have proven that the downward vertical arrow in (2) cannot be multi-valued. Third, the space \mathcal{B}^0 defined by the weaker norm

$$\|\Phi\|_{B^0} \equiv \sum_{A \ni 0} |A|^{-1} \|\Phi_A\|_{\infty} < \infty \qquad (5)$$

arises when the theory is constructed from a variational principle [13,14]. This space is much larger than \mathcal{B}^1 (it admits interactions decaying more slowly with the number of bodies), and exhibits many unphysical features [13,16]. We contend that \mathcal{B}^1 is the largest physically reasonable space of interactions.

3. REGULARITY PROPERTIES

Let us go back to the example of the Ising model. Suppose we are given a measure μ' with a large positive magnetization and a small (but nonzero) correlation length; does this measure come from a Hamiltonian H' with β large and h = 0, or from a Hamiltonian with β not so large (possibly even small) and h large and positive?

One way to decide is to look to the largedeviation properties of the measure μ' . Let Λ be a large cubical box of side L, and let $\mathcal{M}_{\Lambda} \equiv \sum_{x \in \Lambda} \sigma_x$ be the total spin in Λ . Clearly there is an overwhelming probability that \mathcal{M}_{Λ} will be positive; but how rare is it to have \mathcal{M}_{Λ} negative? If μ' is a Gibbs measure for some Hamiltonian with h > 0, then the event $\mathcal{M}_{\Lambda} < 0$ is suppressed by the bulk magnetic field:

$$\operatorname{Prob}_{\mu'}(\mathcal{M}_{\Lambda} < 0) \sim e^{-O(L^d)} . \tag{6}$$

On the other hand, if μ' is a Gibbs measure for some Hamiltonian with h = 0 and $\beta > \beta_c$, then the event $\mathcal{M}_{\Lambda} < 0$ is suppressed only by a *surface* energy:

$$\operatorname{Prob}_{\mu'}(\mathcal{M}_{\Lambda} < 0) \sim e^{-O(L^{d-1})} . \tag{7}$$

It is now easy to decide between the two scenarios for the RG flow. In the starting measure μ_+ , the occurrence of a large region with negative total spin is suppressed only like $e^{-O(L^{d-1})}$; roughly speaking, the measure μ_+ "knows" that it is degenerate with the measure μ_- . But then in the block-spin measure μ'_+ , there must also be a probability $\geq e^{-O(L^{d-1})}$ of observing a negative total spin (since a net negative original spin implies, with high probability, a net negative block spin). Since this contradicts (6), we conclude that μ'_+ cannot be the Gibbs measure of a Hamiltonian with strictly positive magnetic field. Picturesquely, the image measure μ'_+ "remembers" that it arose from an original Hamiltonian H with coexisting phases. Therefore,

It is a relatively short step from these intuitive ideas to a rigorous proof for a general system. The result is [10]:

the RG map cannot be multi-valued.

First fundamental theorem. If μ and ν are Gibbs measures for the same interaction $\Phi \in B^1$, then either the renormalized measures μ' and ν' are both non-Gibbsian, or else there exists an interaction $\Phi' \in B^1$ for which both μ' and ν' are Gibbs measures. In the latter case, Φ' is the *only* interaction (modulo physical equivalence) for which either μ' or ν' is a Gibbs measure. Therefore, the renormalization-group map \mathcal{R} cannot be multi-valued.

If the image measure μ' is Gibbsian, we say that the RG map \mathcal{R} is well-defined at Φ , and we write $\mathcal{R}(\Phi) = \Phi'$.

With a little more work we can prove that the RG map \mathcal{R} is Lipschitz continuous wherever it is well-defined:

Second fundamental theorem. Assume that the RG map \mathcal{R} is well-defined at $\Phi_1, \Phi_2 \in \mathcal{B}^1$, with corresponding renormalized interactions $\Phi'_1, \Phi'_2 \in \mathcal{B}^1$. Then $\|\Phi'_1 - \Phi'_2\|_{\mathcal{B}^0/p.e.} \leq K \|\Phi_1 - \Phi_2\|_{\mathcal{B}^0/p.e.}$, where "/p.e." denotes "modulo physical equivalence". There are two norms involved in this result: the interactions must belong to B^1 — otherwise there is no notion of Gibbs measure — but the norm for the continuity result is the B^0 norm.

In our opinion the discontinuities of RG maps observed in several Monte Carlo studies [3,4,5,6] — *ruled out* by our Fundamental Theorems — are an artifact of the truncation of the renormalized Hamiltonian; for more details, see [10].

4. PATHOLOGIES

Having discussed what cannot go wrong, let us see what can go wrong. In a rather wide variety of examples, the RG map \mathcal{R} is undefined because the image measure μ' is non-Gibbrian.

Note first that, for any Gibbsian measure, the uniform summability $\|\Psi\|_{B^2} < \infty$ implies that the *direct* influence of far-away spins must be areak. More precisely, if we take a volume Λ and then a much larger volume $M \supset \Lambda$, the influence of the spins outside M on observables inside Λ must go to zero as M grows, when the intermediate spins in $M \setminus \Lambda$ are fixed (do not confuse this with the long-range order that can develop when the intermediate spins are not fixed). This property is called guasilocality [14] (or almost-Markovianness [17]). All Gibbs measures are quasilocal, and the converse is almost true [18].

Therefore, a measure is non-quasilocal (hence non-Gibbsian) if there is some mechanism that transmits the information from spins far away through intermediate regions of fixed spins. For many renormalized measures, this mechanism is provided by the original spins if they undergo a phase transition. The key ingredient is the existence of a block-spin configuration ω'_{scaring} such that the constrained system $T^{-1}(\omega'_{special})$ of original spins has several coexisting phases, and in addition these different phases can be selected by an appropriate change of block-spin boundary conditions. In this situation, if the intermediate block spins are fixed in the configuration $\omega'_{special}$, then by changing the block spins arbitrarily far away we can radically alter the behavior of the original spins throughout the lattice, which in turns alters the expectations for block spins close to the ori-

gin. This means that the renormalized (block-spin) measure is non-quasilocal and hence non-Gibbsian. We see that for this to happen, it is not necessary for the original system to be exactly at a firstorder phase transition; it suffices that it be close enough to a first-order transition so that a suitable choice of $\omega'_{special}$ can induce a (first-order) transition in the original-spin system. (Of course, the single configuration $\omega'_{special}$ has probability zero in infinite volume; however, in our examples the argument works also for configurations that agree with $\omega'_{special}$ in large cubes. Such sets of configurations have nonzero probabilities.) All the basic ideas of this argument, and many of the details, are due to Israel [9]; our contribution [10] is to complete and extend his results.

In this fashion we prove non-Gibbsianness at low temperature for the renormalized measures of the following examples [10]: (a) decimation with any spacing $b \ge 2$, for the Ising model in any dimension $d \ge 2$; (b) the Kadanoff transformation for the Ising model in dimension $d \ge 2$, with *small* pand arbitrary block size $b \ge 1$; and (c) the majorityrule transformation with 7×7 blocks for the twodimensional Ising model. Moreover, in dimension $d \ge 3$, the proof of non-Gibbsianness extends to a full neighborhood $\{\beta > \beta_0, |h| < \epsilon(\beta)\}$ of the lowtemperature part of the first-order phase-transition surface.

Though we have not yet been able to demonstrate non-Gibbsianness for other transformations, we feel that the obstacles are technical rather than fundamental. Indeed, in the light of our results, we believe that non-Gibbsianness may be the *normal* situation for RG maps near a first-order phase transition. We emphasize that the non-Gibbsianness discussed here shows up after *only one* renormalization transformation; it is not related with the iteration process itself.

The traditional belief among physicists (including ourselves until recently) is that nearly all physically interesting measures are Gibbsian. The profound message of Israel's pioneering work [9], and of the examples given here [10], is that this traditional belief is false: many physically interesting measures are non-Gibbsian. In fact, we now suspect that Gibbsianness should be considered to be the exception rather than the rule. We expect that many more examples of non-Gibbsianness will be discovered in the near future, particularly in nonequilibrium statistical mechanics [19].

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