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Renormalization Transformations in the Vicinity of First-Order Phase Transitions: What Can and Cannot Go Wrong

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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.

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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 at or near a *first-order* phase transition. On the one hand, the existence of several phases raises the possibility that the RG map may be *discontinuous* or *multivalued* on the first-order transition surface, as the numerical evidence reported by several groups[3–6] seems to suggest. 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;[8] 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-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-Pearce-Israel type. We prove that the RG map, defined on a suitable space of interactions (i.e., 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 $T(\omega \to \omega')$. One can then define a probability distribution $\mu'(\omega')$ of block spins from any given probability distribution $\mu(\omega)$ of original spins:

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

In other words, the RG map is easily defined as 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 Hamiltonians.* That is, μ is chosen as the Gibbs measure for a statistical-mechanical system with Hamiltonian 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 $\mathcal{R}$ on some suitable space of Hamiltonians, by the diagram

$$\begin{array}{ccc} \mu & \xrightarrow{T} & \mu' \\ \uparrow & & \downarrow \\ H & \xrightarrow{R} & H' \end{array} . \quad (2)$$

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

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

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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 $d \geq 2$ 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 $\mu'_\pm$ will have a yet larger magnetization $\pm M'_0$ and a yet smaller correlation length ξ'. We now ask: These image measures $\mu'_\pm$ 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;*[12] in this case the two image measures $\mu'_\pm$ 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 (negative) magnetic field h would get mapped by a single RG step to renormalized Hamiltonians H' having a strictly positive (strictly negative) magnetic field h'. Furthermore, *at $h=0$* the image measures $\mu'_\pm$ would be Gibbsian for *different* Hamiltonians $H'_\pm$ having (among other couplings) magnetic fields of different sign. In this scenario, the RG map $\mathcal{R}$ would be *discontinuous* as one approaches the phase-transition line, and *multivalued* on that line.[13] 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 *cannot* occur: The RG map $\mathcal{R}$ is always single valued and Lipschitz continuous wherever it is defined. On the other hand, in at least some cases[9,10] the first scenario *is not valid either,* because *the Hamiltonian H' fails to exist at all.* That is, *it can occur that the image measure μ' is not a Gibbs measure for any reasonable Hamiltonian.*

General setup.—Our results apply to systems on a lattice $\mathcal{L}=Z^d$ characterized by a single-spin space Ω_0, which comes equipped with a physically natural single-spin 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* $(\Omega'=\Omega_0^{\mathcal{L}'},\mu^{0\prime})$ such that (i) T is a probability kernel; (ii) T carries translation-invariant measures on Ω into translation-invariant measures on Ω'; and (iii) 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 setup 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 $\mu \rightarrow \mu'$ induced by T is always well defined; 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.[14,15] 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 $\Phi_A:\Omega\rightarrow\mathbb{R}$, 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

$$\|\Phi\|_{\mathcal{B}^1} \equiv \sum_{A\ni 0} \|\Phi_A\|_\infty < \infty\,, \tag{4}$$

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

$$H^{\Phi}_{\Lambda,\tau}(\omega) = \sum_{A\cap\Lambda\neq\emptyset} \Phi_A(\omega\wedge\tau)\,, \tag{5}$$

where $\omega\wedge\tau$ is the configuration coinciding with ω inside Λ and with τ outside it. This Hamiltonian is in turn used to define the Boltzmann-Gibbs distribution $\pi^{\Phi}_{\Lambda,\tau}$. 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 $\pi^{\Phi}_{\Lambda,\tau}$.

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[16] have proven that a given measure μ can be Gibbsian for at most one interaction $\Phi\in\mathcal{B}^1$. Third, the space $\mathcal{B}^0$

defined by the weaker norm

$$||\Phi||_{\mathcal{B}^0} \equiv \sum_{A \ni 0} |A|^{-1} ||\Phi_A||_\infty < \infty \tag{6}$$

arises when the theory is constructed from a variational principle.[14,15] 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.[14,17] We contend that $\mathcal{B}^1$ is the largest physically reasonable space of interactions.

Single valuedness and continuity of the RG map. —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 *large-deviation* 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 $\mathcal{M}_\Lambda$ will be positive; but how rare is it to have $\mathcal{M}_\Lambda$ *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:

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

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:

$$\text{Prob}_{\mu'}(\mathcal{M}_\Lambda < 0) \sim e^{-O(L^{d-1})} . \tag{8}$$

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 $\gtrsim e^{-O(L^{d-1})}$ of observing a negative total spin (since a net negative original spin implies, with high probability, a net negative block spin). Since this contradicts (7), 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, the RG map *cannot* be multivalued.

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

First fundamental theorem.— If μ and ν are Gibbs measures for the same interaction $\Phi \in \mathcal{B}^1$, then either the renormalized measures μ' and ν' are both non-Gibbsian, or else there exists an interaction $\Phi' \in \mathcal{B}^1$ 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 multivalued.

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 $||\Phi'_1 - \Phi'_2||_{\mathcal{B}^0/\text{p.e.}} \le K ||\Phi_1 - \Phi_2||_{\mathcal{B}^0/\text{p.e.}}$, where "/p.e." denotes "modulo physical equivalence."

There are two norms involved in this result: The interactions must belong to $\mathcal{B}^1$—otherwise there is no notion of Gibbs measure—but the norm for the continuity result is the $\mathcal{B}^0$ norm.

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

Pathologies in the vicinity of a first-order phase transition.— 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-Gibbsian.*

Note first that, for any Gibbsian measure, the uniform summability $||\Phi||_{\mathcal{B}^1} < \infty$ implies that the *direct* influence of far-away spins must be *weak.* 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 $M \backslash \Lambda$ are *fixed* (do not confuse this with the long-range order than can develop when the intermediate spins are *not* fixed). This property is called *quasilocality*[15] (or almost-Markovianness[18]). All Gibbs measures are quasilocal, and the converse is almost true.[19]

Therefore, a measure is nonquasilocal (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* $\omega'_{special}$ *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 ω'_{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 origin. This means that the renormalized (block-spin) measure is nonquasilocal and hence non-Gibbsian. We see that for this to happen, it is not necessary for the original system to be exactly *at* a first-order phase transition; it suffices that it be *close enough* to a first-order transition so that a suitable choice of ω'_{special} can induce a (first-order) transition in the original-spin system. (Of course, the single configuration ω'_{special} has probability zero in infinite volume; however, in our examples the argument works also for configurations that agree with ω'_{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] we have completed and extended his results.

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

Though we have not yet been able to demonstrate non-Gibbsian character for other transformations, we feel that the obstacles are technical rather than fundamental. Indeed, in the light of our results, we believe that non-Gibbsian character may be the *normal* situation for RG maps near a first-order phase transition. We emphasize that the non-Gibbsian character 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 Gibbsian character should be considered to be the exception rather than the rule. We expect that many more examples of non-Gibbsian character will be discovered in the near future, particularly in nonequilibrium statistical mechanics.[20]

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