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# On the Global Character of Some Restricted Equilibrium Conditions—A Remark on Metastability

**J. Fernando Perez[1,2] and R. H. Schonmann[1,3]**

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For classical lattice systems with finite-range interactions it is proven that if a state minimizes a free-energy functional at nonzero temperature with respect to variations of the state inside all regions of limited size (for instance, all regions with only one lattice site!) then it is a Gibbs state. This result rules out the possibility of defining metastable states at $T \neq 0$ as those which satisfy the thermodynamical stability conditions for regions with small volume-to-surface ratio, unlike the $T = 0$ case.

**KEY WORDS:** Local D.L.R. states; metastability.

## 1. INTRODUCTION

The equilibrium states of lattice systems with finite-range interactions at nonzero temperature can be characterized by the D.L.R. condition(1). This set of equations expresses the requirement that for every finite region the conditional probabilities of the internal configurations given the external configuration are Gibbsian.

The problem of characterization of metastable states of these systems remains largely open in spite of several attempts. In some approaches(2,3) states satisfying a restricted Gibbs condition were shown to display some desirable features(4) of metastable states. The restrictions imposed were in the configuration space of the system and forced the state to be far from the equilibrium one. This paper originated from an attempt to provide a variational principle from which both the stable and metastable states would emerge as the only solutions. The motivation for this search is found

[1] Instituto de Física—Universidade de São Paulo, C. Postal 20.516—São Paulo, S. P., Brazil.
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in the analysis of the ground state of the Ising model with an external field. There one easily sees that if we require that a state minimizes the energy with respect to variations of the state inside arbitrary regions of a "size" smaller than a certain critical value, then there are exactly two solutions: the true ground state and the "metastable" state (see Appendix). At nonzero temperature the natural generalization would consist in looking for states which minimize the free energy with respect again to variations of the state inside arbitrary regions of not too large "size" ("size" stands for the ratio volume/surface). Our results are "no-go" theorems: the only solution of this variational problem at $T \neq 0$ is the true Gibbs state.

This paper is organized as follows. In Section 2 we describe the systems under consideration and show that if a state satisfies the D.L.R. equations for regions containing only one lattice site then it is a Gibbs state. In Section 3 we show that the condition of local thermodynamical stability (L.T.S.)[2b] restricted to a finite region implies the D.L.R. equation for that region. In the Appendix we present for completeness the $T = 0$ case which motivated the whole discussion.

We do not claim complete originality, as some of our results may be known in one form or another. For instance, a version of Theorem 1, under slightly modified assumptions which are not sufficient for our purposes, can be found in Refs. 4 and 5. However, to the best of our knowledge the implications of these results to the theory of metastability have nowhere been discussed.

## 2. RESTRICTED D.L.R. CONDITION

Throughout this paper we will consider a classical lattice system (spin system) with finite-range interactions. At each site $i$ of an infinite lattice $\mathfrak{L}$ (typically $Z^v$, $v = 1, 2, 3, \ldots$) we have a finite state space $\Gamma_i$, which for simplicity we take to be independent of $i$, $\Gamma_i = \Gamma$. A configuration $x$ of this system is a function

$$x: \mathfrak{L} \to \Gamma \qquad i \to x(i) \in \Gamma$$

with $x(i)$ denoting the configuration at the site $i$, i.e., $x \in \Omega = \Gamma^{\mathfrak{L}}$. For a finite region $\Lambda \subset \mathfrak{L}$ we denote by $x_\Lambda$ a configuration "inside $\Lambda$," i.e., a function $x_\Lambda : \Lambda \to \Gamma$, i.e., $x_\Lambda \in \Omega_\Lambda = \Gamma^\Lambda$. Given a configuration $x \in \Omega$ we denote by $x|_\Lambda$ its restriction to $\Lambda$. If $\Lambda_1 \cap \Lambda_2 = \phi$ we denote by $x_{\Lambda_1} x_{\Lambda_2}$ the joint configuration in $\Omega_{\Lambda_1 \cup \Lambda_2}$ i.e., $x_{\Lambda_1} x_{\Lambda_2}(i) = x_{\Lambda_1}(i)$ if $i \in \Lambda_1$ and $x_{\Lambda_1} x_{\Lambda_2}(i) = x_{\Lambda_2}(i)$ if $i \in \Lambda_2$. If $\Lambda_2 \subset \Lambda_1$, then $x_{\Lambda_2}$ is the restriction of $x_{\Lambda_1}$ to $\Lambda_2$.

A state of the system is a probability measure in the measure space $(\Omega, \Sigma)$ where $\Sigma$ is the $\sigma$ field generated by the cylinder sets. Given a state $\mu$ we denote by $p(x_\Lambda)$ the probability that the configuration inside $\Lambda$ is $x_\Lambda$, i.e., $p(x_\Lambda) = \mu(\{x : x|_\Lambda = x_\Lambda\})$.

The interaction is given by a collection $\{\phi_\Lambda, \Lambda \in \mathcal{L}, \Lambda \text{ finite}\}$ of functions $\phi_\Lambda : \Omega_\Lambda \to R$. The interaction is said to have range $R$ if $\phi_\Lambda = 0$ when diameter of $\Lambda > R$. Of course $\phi_\Lambda$ can be considered as function on $\Omega$ via $\phi_\Lambda(x) = \phi_\Lambda(x \mid {}_\Lambda)$. We denote by $H_\Lambda$ the energy in the interior of $\Lambda$, i.e.,

$$H_\Lambda = \sum_{x \subset \Lambda} \phi_x$$

and by $V_\Lambda$ the interaction between sites in $\Lambda$ and in $\Lambda^c$, i.e.,

$$V_\Lambda = \sum_{\substack{x \cap \Lambda \neq \emptyset \\ x \cap \Lambda^c \neq \emptyset}} \phi_x$$

For each finite $\Lambda$ we define

$$\Lambda_\phi = \{ i \in \mathcal{L} : \phi_x \neq 0 \text{ for some } x \ni i, x \cap \Lambda \neq \emptyset \}$$

$$\Delta\Lambda = \Lambda_\phi \mid \Lambda$$

With the above notation a state is said to verify the D.L.R. equation at inverse temperature $\beta < \infty$ if

$$p(x_\Lambda y_{\Lambda'}) = T(x_\Lambda \mid y_{\Delta\Lambda}) p(y_{\Lambda'})$$

for each finite $\Lambda' \supset \Delta\Lambda$, $\Lambda' \cap \Lambda = \emptyset$, where

$$T(x_\Lambda | y_{\Delta\Lambda}) = \frac{\exp[-\beta(H_\Lambda + V_\Lambda)(x_\Lambda y_{\Delta\Lambda})]}{\sum_{z_\Lambda} \exp[-\beta(H_\Lambda + V_\Lambda)(z_\Lambda y_{\Delta\Lambda})]}$$

A state is said to be a (global) D.L.R. state if it verifies the D.L.R. equation for each finite region $\Lambda \subset \mathcal{L}^{(1)}$.

**Definition.** A state is a *restricted* D.L.R. state if it verifies the D.L.R. equations for each region $\Lambda$ of one single site, i.e., $\Lambda = \{i\}$ for some $i \in \mathcal{L}$.

**Theorem 1.** For classical lattice systems with finite-range interactions a restricted D.L.R. state is a (global) D.L.R. state.

For the proof of the theorem we need the following lemma.

**Lemma.** For a restricted D.L.R. state of a classical lattice system at finite inverse temperature $p(x_A) \neq 0$ $\forall x_A \in \Gamma^\Lambda$ for all finite $\Lambda$.

*Proof of the lemma.* We will proceed by induction on the size of the region. Let $|\Lambda| = 1$, then from the restricted D.L.R. condition,

$$p(x_\Lambda) = \sum_{y_{\Delta\Lambda}} p(x_\Lambda y_{\Delta\Lambda}) = \sum_{y_{\Delta\Lambda}} p(y_{\Delta\Lambda}) T(x_\Lambda \mid y_{\Delta\Lambda}) \tag{2.1}$$

since $T(x_\Lambda \mid y_{\Delta\Lambda}) > 0$ and $\sum_{y_{\Delta\Lambda}} p(y_{\Delta\Lambda}) = 1$, $p(y_{\Delta\Lambda}) \geqslant 0$ (2.1) implies $p(x_\Lambda) > 0$.

Let us assume that $p(x_\Lambda) > 0$ for all $\Lambda$ such that $|\Lambda| = N$, $\forall x_\Lambda \in \Gamma^\Lambda$. Let $\Lambda' = \Lambda \cup i$, $i \not\subset \Lambda$, $|i| = 1$, $|\Lambda| = N$, and

$$\tilde{i} = \Delta i / \Lambda$$

If $\tilde{i} = \emptyset$ then $\Delta i \subset \Lambda$ and the restricted D.L.R. equation for $i$ implies

$$p(x_{\Lambda'}) = p(x_i x_\Lambda) = T(x_i \mid x_{\Delta i}) p(x_\Lambda)$$

and since by the induction assumption $p(x_\Lambda) > 0$, we have $p(x_{\Lambda'}) > 0$ in this case.

If $\tilde{i} \neq \emptyset$, $\Delta i \subset \tilde{i} \cup \Lambda$ and

$$p(x_{\Lambda'} y_{\tilde{i}}) = p(x_i x_\Lambda y_{\tilde{i}}) = T(x_i \mid z_{\Delta i}) p(x_\Lambda y_{\tilde{i}}) \tag{2.2}$$

where $z_{\Delta i}$ is the configuration whose restrictions are

$$z_{\Lambda \cap \Delta i} = x_{\Lambda \cap \Delta i} \quad z_{\tilde{i}} = y_{\tilde{i}}$$

Now

$$\sum_{y_{\tilde{i}}} p(x_\Lambda y_{\tilde{i}}) = p(x_\Lambda) > 0$$

therefore $p(x_\Lambda y_{\tilde{i}}) > 0$ for some $y_{\tilde{i}}$. From (2.2) we conclude that some $p(x_{\Lambda'} y_{\tilde{i}}) > 0$ and since $p(x_{\Lambda'}) = \sum_{y_{\tilde{i}}} p(x_{\Lambda'} y_{\tilde{i}})$ we obtain $p(x_{\Lambda'}) > 0$. ■

***Remark.*** Notice that the lemma is false for the ground state ($\beta = \infty$).

***Proof of Theorem 1.*** Given a finite $\Lambda \subset \mathcal{L}$ and a finite $\Lambda' \supset \Delta\Lambda$, $\Lambda' \cap \Lambda = \emptyset$, let $i \subset \Lambda$, $|i| = 1$, $S_i = (\Lambda \cup \Lambda')/i$. Clearly $S_i \supset \Delta i$. Then the restricted D.L.R. condition implies

$$p(x_i y_{S_i}) = p(y_{S_i}) T(x_i \mid y_{\Delta i})$$

Using the lemma

$$\frac{p(x_i y_{S_i})}{p(z_i y_{S_i})} = \frac{T(x_i \mid y_{\Delta i})}{T(z_i \mid y_{\Delta i})} = \frac{\exp\{-\beta[H_i(x_i) + V_i(x_i y_{\Delta i})]\}}{\exp\{-\beta[H_i(z_i) + V_i(z_i y_{\Delta i})]\}}$$

$$= \frac{\exp\{-\beta H_{\Lambda \cup \Lambda'}(x_i y_{S_i})\}}{\exp\{-\beta H_{\Lambda \cup \Lambda'}(z_i y_{S_i})\}}$$

This means that for any two configurations $x_{\Lambda_0}, z_{\Lambda_0}$ of $\Lambda_0 = \Lambda \cup \Lambda'$ which differ just at a single site $i \in \Lambda$,

$$\frac{p(x_{\Lambda_0})}{p(z_{\Lambda_0})} = \frac{\exp[-\beta H_{\Lambda_0}(x_{\Lambda_0})]}{\exp[-\beta H_{\Lambda_0}(z_{\Lambda_0})]}$$

Now given any pair of configurations $x_{\Lambda_0}, z_{\Lambda_0}$ inside $\Lambda_0$ that differ only inside $\Lambda$ we can construct a chain $y_{\Lambda_0}^{(1)}, \ldots, y_{\Lambda_0}^{(N)}$ of configurations in $\Lambda_0$, such that $y_{\Lambda_0}^{(1)} = x_{\Lambda_0}, y_{\Lambda_0}^{(N)} = z_{\Lambda_0}$ with $y_{\Lambda_0}^{(k)}$ differing from $y_{\Lambda_0}^{(k+1)}$, $k = 1, \ldots, N-1$ only at one site inside $\Lambda$. Then

$$\frac{p(x_{\Lambda_0})}{p(z_{\Lambda_0})} = \frac{p\big(y_{\Lambda_0}^{(1)}\big)}{p\big(y_{\Lambda_0}^{(2)}\big)} \cdots \frac{p\big(y_{\Lambda_0}^{(N-1)}\big)}{p\big(y_{\Lambda_0}^{N}\big)} = \frac{\exp[-\beta H_{\Lambda_0}(x_{\Lambda_0})]}{\exp[-\beta H_{\Lambda_0}(z_{\Lambda_0})]} \tag{2.3}$$

The above relation implies the D.L.R. equation for the region $\Lambda$. In fact (2.3) may be rewritten in the form

$$\frac{p(x_\Lambda y_{\Lambda'})}{p(z_\Lambda y_{\Lambda'})} = \frac{\exp[-\beta H_{\Lambda_0}(x_\Lambda y_{\Lambda'})]}{\exp[-\beta H_{\Lambda_0}(z_\Lambda y_{\Lambda'})]} = \frac{\exp[-\beta H_{\Lambda_\phi}(x_\Lambda y_{\Delta\Lambda})]}{\exp[-\beta H_{\Lambda_\phi}(z_\Lambda y_{\Delta\Lambda})]}$$

and since $\sum_{z_\Lambda} p(z_\Lambda y_{\Lambda'}) = p(y_{\Lambda'})$ we get $p(x_\Lambda y_{\Lambda'}) = p(y_{\Lambda'})T(x_\Lambda \mid y_{\Lambda'})$. ■

## 3. RESTRICTED LOCAL THERMODYNAMICAL STABILITY

Following Sewell[2b] we define the free-energy content of a region $\Lambda$ in the state $\mu$ by

$$F_\Lambda(\mu) = \int d\mu_{\Lambda^c}(y_{\Lambda^c}) \sum_{x_\Lambda} \big[ \tilde{\mu}(x_\Lambda \mid y_{\Lambda^c})(H_\Lambda + V_\Lambda)(x_\Lambda y_{\Delta\Lambda})$$
$$+ kT\tilde{\mu}(x_\Lambda \mid y_{\Lambda^c}) \ln \tilde{\mu}(x_\Lambda \mid y_{\Lambda^c}) \big]$$

where $\mu_{\Lambda^c}$ is the restriction of the state to the complement $\Lambda^c$ of $\Lambda$ and $\tilde{\mu}(x_\Lambda \mid y_{\Lambda^c})$ is the conditional probability of $x_\Lambda$ given $y_{\Lambda^c}$.

A state $\mu$ is said to be (globally) L.T.S. if for each finite $\Lambda$

$$F_\Lambda(\mu') \geqslant F_\Lambda(\mu)$$

for all $\mu'$ such that $\mu'_{\Lambda^c} = \mu_{\Lambda^c}$. In other words, the state is L.T.S. if the free-energy content of the state in the region $\Lambda$ is minimum with respect to variations of the state inside $\Lambda$, for all finite $\Lambda$. For finite range interactions L.T.S. implies D.L.R. condition[2b]. The theorem below implies even more.

**Theorem 2.** Let $\Lambda$ be a finite subset of $\mathfrak{L}$ and $\mu$ be a state of a system with finite-range interaction for which $F_\Lambda(\mu') \geqslant F_\Lambda(\mu)$ for all $\mu'$ such that $\mu'_{\Lambda^c} = \mu_{\Lambda^c}$. Then the state $\mu$ verifies the D.L.R. equation for the region $\Lambda$.

***Proof.*** For a given $y_{\Lambda^c}$ let $f_{y_{\Lambda^c}}$ denote the free-energy functional

$$f_{y_{\Lambda^c}}(\mu(x_\Lambda)) = \sum_{x_\Lambda} \big[ \mu(x_\Lambda)(H_\Lambda + V_\Lambda)(x_\Lambda y_{\Delta\Lambda}) + kT\mu(x_\Lambda) \ln \mu(x_\Lambda) \big]$$

It is well known that the unique minimum of this functional is attained at

$$\mu_{y_{\Lambda^c}}(x_\Lambda) = T(x_\Lambda \mid y_{\Delta\Lambda})$$

Let now $\mu$ be a state which minimizes $F_\Lambda$ against variations inside $\Lambda$. Then

$$\tilde{\mu}(x_L \mid y_{\Lambda^c}) = T(x_\Lambda \mid y_{\Delta\Lambda}) \tag{3.1}$$

for almost all $y_{\Lambda^c}$ with respect to $\mu_{\Lambda^c}$. In fact let $E$ be a measurable set of configurations outside $\Lambda$ such that $\tilde{\mu}(x_\Lambda \mid y_{\Lambda^c}) \neq T(x_\Lambda \mid y_{\Delta\Lambda})$ for all $y_{\Lambda^c} \in E$, and let $\nu$ be the state given by

$$\nu(x_\Gamma) = \mu_{\Lambda^c}(x_{\Gamma\cap\Lambda^c}) \sum_{\substack{z_\Lambda \\ z_{\Lambda\cap\Gamma} = x_{\Lambda\cap\Gamma}}} \int d\mu_{\Lambda^c}(y_{\Lambda^c})\delta(y_{\Gamma\cap\Lambda^c} = x_{\Gamma\cap\Lambda^c})T(z_\Lambda \mid y_{\Delta\Lambda}) \tag{3.2}$$

for each finite $\Gamma \subset \mathfrak{L}$.

Notice that the state $\nu$ is equal to $\mu$ when restricted to $\Lambda^c$, and inside $\Lambda$ satisfies (III.1). If $\mu_\Lambda(E) = \nu_\Lambda(E) \neq 0$ then

$$F_\Lambda(\mu) - F_\Lambda(\nu) > 0$$

as the result of integrating a positive function over a set of positive measure. This proves (3.1)

If $\Delta\Lambda \subset \Lambda'$ and $p(y_{\Lambda'}) \neq 0$ then

$$\tilde{\mu}(x_\Lambda \mid y_{\Lambda'}) = \frac{\int_{z\,|\,\Lambda' = y_{\Lambda'}} d\mu_{\Lambda^c}(z_{\Lambda^c})\tilde{\mu}(x_\Lambda \mid z_{\Lambda^c})}{\int_{z\,|\,\Lambda' = y_{\Lambda'}} d\mu_{\Lambda^c}(z_{\Lambda^c})} = T(x_\Lambda \mid y_{\Delta\Lambda})$$

and

$$p(x_\Lambda y_{\Lambda'}) = T(x_\Lambda \mid y_{\Delta\Lambda})p(y_{\Lambda'}) \tag{3.3}$$

If $p(y_{\Lambda'}) = 0$, then $p(x_\Lambda y_{\Lambda'}) = 0$ and (3.3) which is the D.L.R. equation for $\Lambda$, is true too. ■

## APPENDIX—A RESTRICTED VARIATIONAL PRINCIPLE FOR METASTABLE STATES AT $T = 0$

Let us for simplicity consider an Ising model in $Z^\nu$ at $T = 0$ with nearest-neighbor interaction, with a Hamiltonian given formally by

$$H = -J\sum_{\langle ij\rangle} \sigma_i\sigma_j + h\sum_{i\in Z^\nu} \sigma_i$$

where the $\sum_{\langle ij\rangle}$ is the sum over all pairs of nearest-neighbor sites, with $J > 0$, $h > 0$. The ground state of the system is a measure $\mu_-$ concentrated in the configuration $x_-$ with all spins down, i.e., $x_-(i) = -1$, $\forall i \in Z^\nu$:

$$\mu_-(E) = 1, \qquad x_- \in E \in \sum$$

$$\mu_-(E) = 0, \qquad x_- \notin E \in \sum$$

If $0 < h < 2\nu J$ then the state $\mu_+(E) = \mu_-(-E)$ is the "metastable state" and verifies the following variational principle: for all regions $\Lambda$ such that $h|\Lambda| \leqslant 2\nu J|\partial\Lambda|$ where $|\Lambda|$ and $|\partial\Lambda|$ are the volume and surface of $\Lambda$, respectively,

$$F_\Lambda(\mu') \geqslant F_\Lambda(\mu_+)$$

for all $\mu'$ such that $\mu'_\Lambda = \mu_{+\Lambda^c}$ as one trivially verifies. Here $F_\Lambda(\mu)$ is as defined in Section 3 for $T = 0$.

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## REFERENCES

1. R. L. Dobrushin, *Theor. Prob. Appl.* **13**:201 (1968); *Funct. Anal. Appl.* **2**:31 and 44 (1968); O. E. Lanford III and D. Ruelle, *Commun. Math. Phys.* **13**:194 (1969).
2. (a) O. Penrose and J. L. Lebowitz, Towards a rigorous molecular theory of metastability, in *Studies in Statistical Mechanics*, Vol. 7, E. W. Montroll and J. L. Lebowitz, eds. (North-Holland, Amsterdam 1979), pp. 293–240; (b) G. L. Sewell, Stability, equilibrium and metastability in statistical mechanics, *Phys. Rep.* **57**:307–342 (1980).
3. D. Capocaccia, M. Cassandro, and E. Olivieri, *Commun. Math. Phys.* **39**:185 (1974).
4. F. Spitzer, *Random Fields and Interacting Particle Systems*, (Mathematical Association of America, Oberlin, Ohio 1971).
5. E. Presutti, Lectures notes in statistical mechanics, Universidade de São Paulo, 1979 (unpublished).