INSTITUTO DE FÍSICA

preprint

IFUSP/P-294

ON THE GLOBAL CHARACTER OF SOME RESTRICTED EQUILIBRIUM CONDITIONS - A REMARK ON METASTABILITY

by

J. Fernando Perez and R.H.Schonmann

Instituto de Física - Universidade de São Paulo

UNIVERSIDADE DE SÃO PAULO
INSTITUTO DE FÍSICA
Caixa Postal - 20.516
Cidade Universitária
São Paulo - BRASIL

ON THE GLOBAL CHARACTER OF SOME RESTRICLED EQULIBRIUM CONDITIONS - A REMARK ON METASTABILITY

J. Fernando Perez* and R.H.Schonmann**
Instituto de Física - Universidade de São Paulo
C.Postal 20.516 - São Paulo, S. P.,
Brasil

ABSTRACT

For classical lattice systems with finite range interactions it is proven that if a state minimizes a free-energy functional at non-zero 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≠0 as those which satisfy the thermodynamical stability conditions for regions with small volume to surface ratio, unlike the T=0 case.

* Partial financial support by CNPq.

** Financial support by FAPESP.

SEP/81

I. INTRODUCTION

The equilibrium states of lattice systems with finite range interactions at non-zero temperature can be characterized by the D.L.R. condition [1]. This set of equations expresses the requirement that for every finite region the conditionl probability of the internal configurations given the external configuration are Gibbsian.

The problem of characterization of metastable states of these systems in spite of several attempts remains largely open. 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 enforced 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 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 non-zero temperature the natural generalization would consist in looking for states which minimizes 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 solutions of this variational principle at T≠0 is the true Gibbs state.

This paper is organized as follows. In section II 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 III 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 completness 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.[4,5]. However to the best of our knowledge the implications of these results to the theory of metastability have nowhere been discussed.

II. RESTRICTED DLR CONDITION

All along this article we will consider a classical lattice system (spin system) with finite range interactions. At each site i of an infinite lattice $\mathcal{L}$ (typically Z^{ν}, $\nu=1,2,3,\ldots$) we have a finite state space Γ_i, wich for simplicity we take to be independent of i, $\Gamma_i=\Gamma$. A configuration x of this system is a function

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

with x(i) denoting the configuration at the site i, ie, $x \in \Omega = \Gamma^{\mathcal{L}}$. For a finite region $\Lambda \subset \mathcal{L}$ we denote by x_Λ a configuration "inside Λ" 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 Λ. 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 $x_{\Lambda_1} x_{\Lambda_2}(i) = x_{\Lambda_2}(i)$ $i \in \Lambda_2$. If $\Lambda_2 \subset \Lambda_1$, then x_{Λ_2} is the restriction of x_{Λ_1} to Λ_2.

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

The interaction is given by a collection $\{\phi_\Lambda, \Lambda \in \mathcal{L}, \Lambda$ 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 ϕ_Λ can be considered as function on Ω via $\phi_\Lambda(x) = \phi_\Lambda(x|_\Lambda)$. We denote by H_Λ the energy in the interior of Λ, i.e.

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

and by V_Λ the interaction between sites in Λ and in Λ^c, i.e.

$$V_\Lambda = \sum_{\substack{x \cap \Lambda \neq 0 \\ x \cap \Lambda \neq 0}} \phi_x$$

For each finite Λ we define

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

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

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

for each finite $\Lambda' \supset \Delta\Lambda$, $\Lambda' \cap \Lambda = \phi$, 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 $\Lambda \subset \mathcal{S}$ [1].

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

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 $p(x_\Lambda) \neq 0\ \forall\, x_\Lambda\ \Gamma^\Lambda$ for all finite Λ.

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.

$$p(x_\Lambda) = \sum_{y_{\Delta\Lambda}} p(x_\Lambda y_{\Delta\Lambda}) = \sum_{y_{\Delta\Lambda}} p(y_{\Delta\Lambda}) T(x_\Lambda | y_{\Delta\Lambda}) \qquad \text{(II.1)}$$

since $T(x_\Lambda | y_{\Delta\Lambda}) > 0$ and $\sum_{y_{\Delta\Lambda}} p(y_{\Delta\Lambda}) = 1$, $p(y_{\Delta\Lambda}) \geq 0$ (II.1) implies $p(x_\Lambda) > 0$.

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

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

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

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

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

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

$$p(x_{\Lambda'} y_{\tilde{i}}) = p(x_i x_\Lambda y_{\tilde{i}}) = T(x_i | z_{\Delta i}) p(x_\Lambda y_{\tilde{i}}) \qquad \text{(II.2)}$$

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

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

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 (II.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 $\Lambda \subset \mathcal{S}$ and a finite $\Lambda' \supset \Delta\Lambda$, $\Lambda' \cap \Lambda = \phi$, let $i \subset \Lambda$, $|i| = 1$, $S_i = (\Lambda \cup \Lambda')/i$. Clarly $S_i \supset \Delta i$. Then the restricted D.L.R. condition implies

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

Using the lemma

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

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

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

$$\frac{p(x_{\Lambda_o})}{p(z_{\Lambda_o})} = \frac{\exp\{-\beta H_{\Lambda_o}(x_{\Lambda_o})\}}{\exp\{-\beta H_{\Lambda_o}(z_{\Lambda_o})\}}$$

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

$$\frac{p(x_{\Lambda_o})}{p(z_{\Lambda_o})} = \frac{p(y^{(1)}_{\Lambda_o})}{p(y^{(2)}_{\Lambda_o})} \cdots\cdots \frac{p(y^{(N-1)}_{\Lambda_o})}{p(y^{N}_{\Lambda_o})} = \frac{\exp\{-\beta H_{\Lambda_o}(x_{\Lambda_o})\}}{\exp\{-\beta H_{\Lambda_o}(z_{\Lambda_o})\}} \qquad \text{(II.3)}$$

The above relation implies de D.L.R. equation for the region . In fact (II.3) may be rewritten in the form

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

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

III. RESTRICTED LOCAL THEMODYNAMICAL STABILITY

Following Sewell [2b] we define the free energy content of a region Λ in the state μ by

$$F_\Lambda(\mu) = \int d\mu_{\Lambda^c}(y_{\Lambda^c}) \sum_{x_\Lambda} \{\tilde\mu(x_\Lambda|y_{\Lambda^c})(H_\Lambda+V_\Lambda)(x_\Lambda y_{\Delta\Lambda}) +$$

$$+ kT\tilde\mu(x_\Lambda|y_{\Lambda^c})\ln\tilde\mu(x_\Lambda|y_{\Lambda^c})\}$$

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

A state μ is said to be (globally) L.T.S. if for each finite Λ

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

for all μ' 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 Λ is minimum with respect to variations of the state inside Λ, for all finite Λ. For finite range interactions L.T.S. implies D.L.R. condition [2b]. The theorem below implies even more.

<u>Theorem 2</u>: Let Λ be a finite subset of $\mathcal{S}$ and μ be a state of a system with finite range interaction for which $F_\Lambda(\mu') \geq F_\Lambda(\mu)$ for all μ' such that $\mu'_{\Lambda^c} = \mu_{\Lambda^c}$. Then the state μ verifies the D.L.R. equation for the region Λ.

<u>Proof</u>: For a given y_{Λ^c} let $f_{y_{\Lambda^c}}$ denote the free-energy functional

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

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

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

Therefore given a state μ, if it minimizes F_Λ against variations inside Λ

$\tilde{\mu}(x_\Lambda | y_{\Lambda^c}) = T(x_\Lambda | y_{\Delta\Lambda})$ for allmost all y_{Λ^c}. If $\Delta\Lambda \subset \Lambda'$ and $p(y_{\Lambda'}) \neq 0$ then

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

and $$p(x_\Lambda y_{\Lambda'}) = T(x_\Lambda | y_{\Delta\Lambda})\, p(y_{\Lambda'}) \qquad \text{(III.1)}$$

If $p(y_{\Lambda'}) = 0$, then $p(x_\Lambda y_{\Lambda'}) = 0$ and (III.1) which is the D.L.R. equation for Λ is true too.

APPENDIX - A RESTRICTED VARIATIONAL PRINCIPLE FOR METASTABLE STATES AT T=0.

Let for simplicity consider an Ising Model in Z^ν at T=0 with nearest neighbor interaction, with a hamiltonian given formally by

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

where the $\sum_{<ij>}$ is the sum over all pairs of nearest neighbor sites,

with J>0, h>0. The ground state of the system is a measure μ_- concentrated in the configuration x_- with all spins down, i.e. $x_-(i)=-1, \forall\, i \in Z^\nu$:

$$\mu_-(E)=1, \quad x_- \in E \in \Sigma$$
$$\mu_-(E)=0, \quad x_- \notin E \in \Sigma .$$

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 Λ such that $h|\Lambda| \leq 2\nu J|\partial\Lambda|$ where $|\Lambda|$ and $|\partial\Lambda|$ are the volume and surface of Λ respectively

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

for all μ' s.t. $\mu'_{\Lambda^c} = \mu_{+\Lambda^c}$ as one trivially verifies. Here $F_\Lambda(\mu)$ is as defined in section III for T=0.

REFERENCES

(1) R.L.Dobrushin, Theor.Prob.and Appl. 13, 201 (1968) and Funct. Anal. and Appl. 2, 31 and 44 (1968); O.E.Landford III, D. Ruelle, Commun.Math.Phys. 13, 194 (1969).

(2) For reviews see a) O.Penrose and J.L.Lebowitz: "Towards a rigorous molecular theory of metastability", p.293-240 in Studies in Statistical Mechanics, Vol.7; Ed. E.W.Montrall and J.L. Lebowitz, North Holland, 1979. b) G.L.Sewell: "Stability, equilibrium and metastability in Statistical Mechanics", Phys.Rep. 57, 307-342 (1980).

(3) D.Capocaccia, M.Cassandro, E.Olivieri, Commun.Math.Phys. 39, 185 (1974).

(4) F.Spitzer, "Random Fields and Interacting Particle Systems, published by the Mathematical Association of America (1971).

(5) E.Presutti, Lectures Notes in Statistical Mechanics, Universidade de São Paulo, 1979 (unpublished).