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# An approach to metastability in some ferromagnetic systems

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*Abstract.* We propose a new method of defining metastable states of classical statistical mechanical systems, which is based upon an earlier analysis of metastable states of molecules by one of us. Our method allows a computation of the lifetime of the metastable states obtained and conforms to the criteria for metastability of Penrose and Lebowitz, but has the additional feature of providing a strong link with thermodynamics. This link is investigated for some ferromagnetic interactions, and completely analyzed in the van der Waals limit.

## 1. Introduction

Penrose and Lebowitz proposed [1, 2] to calculate the static properties of metastable states from appropriate ensembles chosen according to criteria characterizing metastability. The particular ensembles that they considered were obtained by restricting the set of possible configurations in phase space. Adopting the same general view point as Penrose and Lebowitz, we develop here another approach to the definition of metastable states, which depends upon minimizing the free energy while also controlling the density fluctuations of the states. This definition is of a thermodynamic nature, although consideration of the density fluctuations forces us to formulate the basic quantities in a statistical mechanical manner. Then we study the evolution of our metastable states and show that for suitable values of the thermodynamic parameters, the life time is large.

This approach to metastability is very general and extends to statistical mechanics concepts which were introduced by one of us [3, 4] to analyze metastable states of molecules. In particular it does not involve direct configuration space considerations and therefore could be applied as well to quantum mechanical systems. (For a review and a discussion of various criteria characterizing metastability, see [2, 5].) In a subsequent paper [19], we shall present results which establish a precise connection between our approach to metastability and that of [1, 2], as well as some results concerning the important issue of the formation of metastable states.

In this paper, we shall consider only ferromagnetic classical lattice systems for which the literature is richer and allows comparison with rigorous earlier work on the subject [6]. Glauber dynamics will be used to investigate the dynamical aspects of our metastable states.

The basis of our method is that we minimize the free energy $\mathcal{F}$ under a constraint $\mathcal{W}$ on the second order magnetization fluctuations. If $X$ is the convex set of mixed states of the system and the Hamiltonian in an external field $\mu > 0$ is $H_0 - \mu M$, $M$ being the total magnetization observable, then the free energy

$$\mathcal{F}(\rho) = \operatorname{tr}[(H_0 - \mu M)\rho] - \beta^{-1}\mathcal{S}(\rho)$$

with

$$\mathcal{S}(\rho) = -\operatorname{tr}(\rho \log \rho)$$

is a strictly convex function of $\rho \in X$ [1]). We shall give a definition of the total magnitude $\mathcal{W}(\rho)$ of the second order fluctuations of $\rho$ which has the property that $\mathcal{W}(\rho)$ is a continuous concave function of $\rho$. We then *define* metastable states to be local minima of $\mathcal{F}(\rho)$ subject to a constraint of the form $\mathcal{W}(\rho) \leq K$. The exact appropriate value of $K$ is not specified and will be discussed in Section 4, but $K$ must be of the same order of magnitude as $\mathcal{W}(\rho_\beta)$, where $\rho_\beta$ is the Gibbs state of the system. Moreover, for non-triviality, we must have $K < \mathcal{W}(\rho_\beta)$.

If $\rho'_\beta$ is a local minimum of $\mathcal{F}(\rho)$ under the above constraint, then

$$\mathcal{F}(\rho'_\beta) > \mathcal{F}(\rho_\beta)$$

The function $\mathcal{F}(\rho)$ is then convex and strictly increasing on the interval

$$\{(1-\lambda)\rho_\beta + \lambda\rho'_\beta : 0 \leq \lambda \leq 1\} \subseteq X$$

while $\mathcal{W}(\rho)$ is a continuous concave function on this interval. Simple graphical considerations show that any local minimum of $\mathcal{F}(\rho)$ subject to $\mathcal{W}(\rho) \leq K$ occurs when $\mathcal{W}(\rho) = K$.

We thus have to determine the local minima of $\mathcal{F}(\rho)$ subject to $\mathcal{W}(\rho) = K$, and the method of variation of parameters leads one to a determination of the stationary points of the functional

$$\mathcal{E}(\rho) = \mathcal{F}(\rho) + \alpha\mathcal{W}(\rho)$$

where $\alpha$ is an 'undetermined' multiplier. One finds such stationary points and then fixes $\alpha$ by putting $\mathcal{W}(\rho(\alpha)) = K$.

A detailed analysis of the stationary points of $\mathcal{E}(\rho)$ has been carried out in [3, 4] for the case of a small fixed number of quantum particles, and we can adapt the methods of that paper to our present problem. Because of our particular definition of $\mathcal{W}(\rho)$, it turns out to be linear on the sections

$$X_x = \{\rho \in X : \operatorname{tr}(M\rho) = x\}$$

of $X$, say

$$\mathcal{W}(\rho) = \operatorname{tr}(V_x\rho)$$

for $\rho \in X_x$. Then for $\rho \in X_x$ one has

$$\mathcal{E}(\rho) = \operatorname{tr}[(H_0 - \mu M + \alpha V_x)\rho] - \beta^{-1}\mathcal{S}(\rho)$$

which is a strictly convex function of $\rho$. Thus there is a unique stationary point of

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[1]) All considerations made in the Introduction concern finite volume systems. Although dealing with classical systems, we keep the notation trace for summations on configuration space.

$\mathscr{E}(\rho)$ within $X_x$, which is a minimum and given explicitly by

$$\rho_x = \exp[-\beta(H_0 - \nu M + \alpha V_x)]/\mathrm{tr}\exp[-\beta(H_0 - \nu M + \alpha V_x)]$$

where $\nu$ is determined by

$$\mathrm{tr}(M\rho_x) = x$$

One then defines the function $E$ of the single real variable $x$ by

$$E(x) = \mathscr{E}(\rho_x) \tag{1.1}$$

and looks for solutions of $E'(x) = 0$. Each such solution provides a candidate $\rho_x$ for a metastable state.

We now specify the particular model we shall study. We consider a classical spin system on a square $d$-dimensional lattice with periodic boundary conditions, and $d \geq 2$. The finite volume Hamiltonian $H_0^\Lambda$ on the region

$$\Lambda = \{i = (n_1, \ldots, n_d) : 0 \leq n_r < N\}$$

of volume $|\Lambda| = N^d$ is taken to be

$$H_0^\Lambda = -\sum_{i,j \in \Lambda} h(i-j)\sigma_i\sigma_j$$

We assume that $h \geq 0$, $h(i) > 0$ when $i$ is a nearest neighbour of the origin, and

$$\|h\|_1 = \sum_{i \in \mathbf{Z}^d} h(i) < \infty$$

for thermodynamic stability.

If $M = \sum_i \sigma_i$, then the free energy

$$\begin{aligned}\phi_0^\Lambda(\mu) &= |\Lambda|^{-1} \min\{\mathrm{tr}[(H_0 - \mu M)\rho] - \beta^{-1}\mathscr{S}(\rho)\} \\ &= -(\beta|\Lambda|)^{-1} \log \mathrm{tr}\exp[-\beta(H_0 - \mu M)]\end{aligned}$$

is a concave function of the external field $\mu$. By the Lee-Yang theorem its thermodynamic limit

$$\phi_0(\mu) = \lim_{|\Lambda| \to \infty} \phi_0^\Lambda(\mu)$$

is analytic for $\mu \neq 0$. There is a critical temperature $\beta_0^{-1}$ at which spontaneous magnetization occurs and we assume that $\beta > \beta_0$ throughout. The spontaneous magnetization is denoted by $m_0 > 0$.

The choice of the non-linear functional $\mathscr{W}(\rho)$ is motivated by the following physical considerations. The metastable states are obtained by limiting the fluctuations of the magnetization on a certain scale $\gamma$ which should correspond to the critical size in the droplet model for condensation.

Introducing the spin wave observables

$$\tilde{\sigma}_k = N^{-d/2} \sum_{j \in \Lambda} \exp(ik \cdot j)\sigma_j$$

we shall consider second order fluctuation functionals of the form

$$\mathcal{W}(\rho)=\sum_{k} \tilde{w}_k\langle|\tilde{\sigma}_k-\langle\tilde{\sigma}_k\rangle_\rho|^2\rangle_\rho$$

where the non-negative numbers $\tilde{w}_k$ will control the size of the spin wave fluctuations with wave number $k$. Typically we should choose $\tilde{w}_k=0(1)$ for $|k|<\pi/\gamma$ and $\tilde{w}_k\simeq 0$ for $|k|\geq\pi/\gamma$.

However, there is no need at this point to make a particular choice of the $\tilde{w}_k$. We define generally $\mathcal{W}(\rho)$ by

$$\mathcal{W}(\rho)=\sum_{i,j\in\Lambda} w(i-j)\langle(\sigma_i-\langle\sigma_i\rangle_\rho)(\sigma_j-\langle\sigma_j\rangle_\rho)\rangle_\rho$$

where $w$ is a function on $\mathbf{Z}^d$, independent of $\Lambda$. We will impose only the crucial condition that

$$\hat{w}_k=\sum_{j=\mathbf{Z}^d} w(j)\exp(ik\cdot j)\geq 0 \tag{1.2}$$

for all $k\in\mathbf{R}^d$, ensuring that

$$\mathcal{W}(\rho)\geq 0 \quad \text{for all} \quad \rho.$$

Moreover, we assume for convenience that

$$w(j)\geq 0, \qquad \sum_j w(j)=1$$

In this paper, we shall only develop a theory of translation invariant metastable states. A theory of non translation invariant metastable states is in principle possible, but will not be pursued her.

For this purpose, we introduce translation invariance already for finite volume setting $\sigma_{i+jN}=\sigma_i$ for $i\in\Lambda$, $j\in Z^d$ and using periodic boundary conditions for $H_0^\Lambda$, namely

$$H_0^\Lambda=\sum_{i,j\in\Lambda} h_p(i-j)\sigma_i\sigma_j$$

where

$$h_p(i)=\sum_{j\in Z^d} h(i+jN).$$

It is also convenient to define the constraint $\mathcal{W}(\rho)$ in the same way

$$\mathcal{W}^\Lambda(\rho)=\sum_{i,j\in\Lambda} w_p(i-j)\langle(\sigma_i-\langle\sigma_i\rangle_\rho)(\sigma_j-\langle\sigma_j\rangle_\rho)\rangle_\rho$$

with

$$w_p(i)=\sum_{j\in Z^d} w(i+jN)$$

It is obvious that

$$w_p(i) \geq 0, \qquad \sum_{j \in \Lambda} w_p(i) = 1$$

Moreover, (1.2) implies that the Fourier transform of $w_\rho(i)$ on $\Lambda$ satisfies also

$$\hat{w}_\rho(k) = \sum_{j \in \Lambda} w_p(j) \exp(2i\pi j \cdot k/N) \geq 0 \quad \text{for all} \quad k \in Z^d$$

Thus we have

$$\mathcal{W}^\Lambda(\rho) \geq 0 \text{ for all } \rho \text{ and all } \Lambda. \tag{1.3}$$

From now on, we shall drop the index $\Lambda$ in $H_0^\Lambda$ and $\mathcal{W}^\Lambda(\rho)$ understanding that we use the periodic boundary conditions defined above.

In looking for local minima of

$$\mathscr{E}^\Lambda(\rho) = |\Lambda|^{-1}\{\text{tr}[(H_0 - \mu M)\rho] - \beta^{-1}\mathscr{S}(\rho) + \alpha \mathcal{W}(\rho)\}$$

we shall always suppose that $\rho$ lies in the convex set $X$ of probability measures on the configuration space $2^\Lambda$ which are translation invariant modulo the periodic boundary conditions.

The local minima of $\mathscr{E}^\Lambda$ within $X$ will be called the metastable states of our theory. $\mathscr{E}^\Lambda$ as well as the metastable states depend on a choice of $\alpha$ and $w$. Since these states cannot be exactly stationary under the Glauber dynamics (defined with respect to $H_0 - \mu M$) one does not expect a completely canonical choice for $\alpha$, $w$. One should instead obtain a family of physically similar states for $\alpha$, $w$ with suitable properties. In particular, in order to have metastable states with very slow decay one should fix $\alpha$, $w$ in such a way as to maximize the life time. We defer further discussion of these points to Section 4. Let us add that such non-uniqueness is a common feature of all microscopic theories of metastability existing at present.

We next introduce some further notation. We define the interactions

$$V = \sum_{i,j \in \Lambda} w_p(i-j)\sigma_i\sigma_j$$

and

$$\begin{aligned} V_x &= \sum_{i,j \in \Lambda} w_p(i-j)(\sigma_i - x)(\sigma_j - x) \\ &= V - 2xM + x^2 |\Lambda| \end{aligned} \tag{1.4}$$

We put

$$H = H_0 + \alpha V$$

and let $\phi^\Lambda(\nu)$ be the corresponding finite volume free energy functional for the external field $\nu$, so that

$$\begin{aligned} \phi^\Lambda(\nu) &= |\Lambda|^{-1} \min\{\text{tr}[(H - \nu M)\rho] - \beta^{-1}\mathscr{S}(\rho)\} \\ &= -(\beta |\Lambda|)^{-1} \log \text{tr} \exp[-\beta(H - \nu M)] \end{aligned}$$

If we parametrize the free energy by the magnetization $x$ instead of the external field $\nu$ we obtain

$$\psi^\Lambda(x)=|\Lambda|^{-1}\min\{\mathrm{tr}\,[H\rho]-\beta^{-1}\mathcal{S}(\rho):\mathrm{tr}\,[\sigma_i\rho]=x\}$$
$$=\phi^\Lambda(\nu)+\nu x$$

where $\nu\in\mathbf{R}$ is determined by

$$\frac{\partial\phi^\Lambda}{\partial\nu}(\nu)=-x \tag{1.5}$$

In finite volume $\phi^\Lambda$ and $\psi^\Lambda$ are both analytic functions, $\phi^\Lambda$ is strictly concave and $\psi^\Lambda$ is strictly convex. In terms of these functions, we have

$$\begin{aligned}E^\Lambda(x)&=|\Lambda|^{-1}\min\{\mathrm{tr}\,[(H_0-\mu M)\rho]-\beta^{-1}\mathcal{S}(\rho)+\alpha\mathcal{W}(\rho):\mathrm{tr}\,(\sigma_i\rho)=x\}\\&=|\Lambda|^{-1}\min\{\mathrm{tr}\,[(H_0-\mu M+\alpha V_x)\rho]-\beta^{-1}\mathcal{S}(\rho):\mathrm{tr}\,(\sigma_i\rho)=x\}\\&=\psi^\Lambda(x)-\mu x-\alpha x^2\\&=\phi^\Lambda(\nu)+\nu x-\mu x-\alpha x^2\end{aligned} \tag{1.6}$$

where the ‘effective field’ $\nu$ is determined by (1.5).

The function $E^\Lambda(x)$ is closely related to another functional defined in [4], namely

$$\begin{aligned}F^\Lambda(x)&=|\Lambda|^{-1}\min\{\mathrm{tr}\,[(H_0-\mu M+\alpha V_x)\rho]-\beta^{-1}\mathcal{S}(\rho)\}\\&=\phi^\Lambda(\mu+2\alpha x)+\alpha x^2\end{aligned} \tag{1.7}$$

The following Lemma is analogous to Lemma 10, Lemma 14 and Theorem 15 of [4].

**Lemma 1.** *$E^\Lambda$ and $F^\Lambda$ have the following properties*

(i) *$E^\Lambda(x)+\alpha x^2$ is convex.*
(ii) *$F^\Lambda(x)-\alpha x^2$ is concave.*
(iii) *$E^\Lambda(x)\geq F^\Lambda(x)$ for all $x$.*
(iv) *The following are equivalent*

(a) $E^\Lambda(x)=F^\Lambda(x)$

(b) $\dfrac{\partial E^\Lambda}{\partial x}=0$

(c) $\dfrac{\partial F^\Lambda}{\partial x}=0$

*Proof*

(i) This follows from the convexity of $\psi^\Lambda(x)$.
(ii) This follows from the concavity of $\phi^\Lambda(\nu)$.
(iii) This is immediate since one is minimizing the same expression, but subject to the constraint $\mathrm{tr}\,[\sigma_i\rho]=x$ in the case of $E^\Lambda(x)$.
(iv) (a) One may write

$$\begin{aligned}&F^\Lambda(x)-F^\Lambda(x)\\&=\phi^\Lambda(\nu)-\phi^\Lambda(\mu+2\alpha x)+\nu x-\mu x-2\alpha x^2\\&=\phi^\Lambda(\nu)-\phi^\Lambda(\mu+2\alpha x)+(\mu+2\alpha x-\nu)\frac{\partial\phi^\Lambda}{\partial\nu}(\nu)\end{aligned}$$

By the strict concavity of $\phi^\Lambda$ this is non-negative and equal to zero if and only if

$$\mu + 2\alpha x = \nu \tag{1.8}$$

(b) Differentiating (1.6) yields

$$\frac{\partial E^\Lambda}{\partial x}\frac{dx}{d\nu} = \frac{\partial \phi^\Lambda}{\partial \nu} + x + \nu\frac{d\nu}{dx} - \mu\frac{dx}{d\nu} - 2\alpha x\frac{dx}{d\nu}$$

from which we deduce using (1.5) that

$$\frac{\partial E^\Lambda}{\partial x} = \nu - \mu - 2\alpha x$$

so that $\partial E^\Lambda/\partial x = 0$ is equivalent to (1.8).
(c) Differentiating (1.7) yields

$$\begin{aligned}\frac{\partial F^\Lambda}{\partial x} &= \frac{\partial \phi^\Lambda(\mu+2\alpha x)}{\partial(\mu+2\alpha x)}2\alpha + 2\alpha x\\ &= 0\end{aligned}$$

if and only if

$$\frac{\partial \phi^\Lambda(\mu+2\alpha x)}{\partial(\mu+2\alpha x)} = -x$$

By (1.5) and the strict concavity of $\phi^\Lambda$ this is equivalent to (1.8).

## 2. Thermodynamics

In the above analysis, and in our later treatment of the dynamics, we have to consider a finite volume system, but for the thermodynamics it is much easier to study the system only in the thermodynamic limit. We therefore define

$$E(x) = \psi(x) - \mu x - \alpha x^2 \tag{2.1}$$

$$F(x) = \phi(\mu + 2\alpha x) + \alpha x^2 \tag{2.2}$$

with

$$\psi(x) = \lim_{|\Lambda|\to\infty} \psi^\Lambda(x) \quad \text{and} \quad \phi(\nu) = \lim_{|\Lambda|\to\infty} \phi^\Lambda(\nu).$$

We note that these functions still satisfy properties (i)–(iii) of Lemma 1. The inequality (1.3) implies that

$$E^\Lambda(x) \geq \psi_0^\Lambda(x) - \mu x$$

for all $x$, from which we deduce that

$$E(x) \geq \psi_0(x) - \mu x \tag{2.3}$$

Our goal in this section is to obtain as much information as possible concerning the form of $E(x)$.

We shall see that for small $\mu>0$, $E(x)$ has a global minimum, corresponding to the Gibbs state, near $x=m_0$, and a local minimum, corresponding to the metastable state near $x=-m_0$. Moreover, the convex envelope of $E(x)$ is approximately equal to $\psi_0(x)-\mu x$ for all $x\in(-1,1)$ so that $E(x)$ is a candidate for a 'modified' free energy functional as in the van der Waals theory of condensation. In fact, we will see in Section 5 that in the van der Waals limit $E(x)$ coincide essentially with the usual (non-convex) functional of the mean field theory. The general picture we shall obtain is

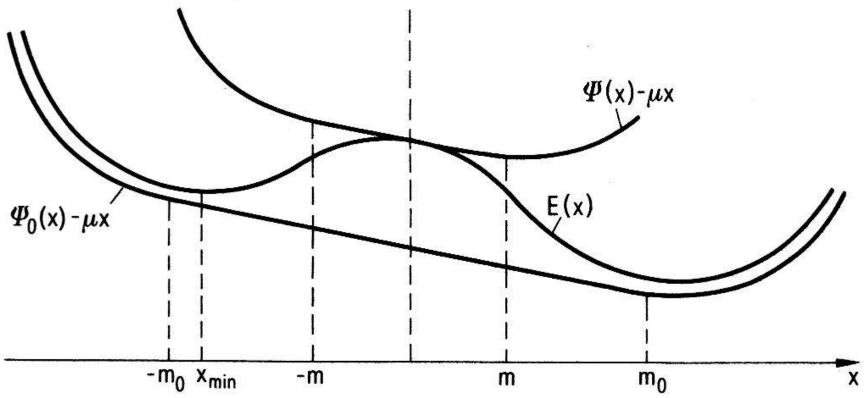


Figure 1

The study of $E(x)$ depends upon information concerning the thermodynamic function $\psi(x)$ and $\phi(\nu)$ associated with the Hamiltonian $H=H_0+\alpha V$, i.e. belonging to a ferromagnetic system perturbed by the small antiferromagnetic term $\alpha V$. Because of the incomplete nature of the literature on such systems, we shall rely here upon a number of hypotheses concerning the properties of these thermodynamic functions, but to our knowledge all existing rigorous results support the correctness of these hypotheses. The hypotheses express that below the critical temperature of $H_0$ and if the perturbation is sufficiently small, $H_0+\alpha V$ should still have the typical ferromagnetic properties. In an appendix we gather together conditions on $h$ and $w$ under which the hypotheses may be valid. Our first three hypotheses are

(H1) For small enough $\alpha>0$ the spontaneous magnetization $m$ of $H$ satisfies $0<m<m_0$. Moreover, for fixed $w$, $m\to m_0$ as $\alpha\to 0$.

(H2) For small enough $\alpha>0$ one has

$$\psi(x)=f \quad \text{for} \quad -m\le x\le m$$

where $f$, $m$ depend on $\alpha$, $w$. Moreover $\psi(x)$ is analytic for $|x|>m$ and differentiable at $x=\pm m$ with $\psi'(\pm m)=0$.

(H3) For small enough $\alpha>0$ the magnetization $x(\nu)$ for the Hamiltonian $H$ in the external field $\nu$ is a concave function of $\nu$.

**Theorem 2.** *If* (H1) *and* (H2) *hold, and*

$$2\alpha m>\mu \tag{2.4}$$

*then $E(x)$ has a local minimum in the region $x<-m$. If* (H3) *also holds then this minimum is unique.*

*Proof.* By (H2) we see that $E(x)$ is a differentiable function of $x \in (-1, 1)$, and that

$$E'(-m) = -\mu + 2\alpha m$$

so that (2.4) is equivalent to $E'(-m)<0$. The existence of a local minimum follows by combining this with the inequality

$$E(x) \geq f_0 - \mu x$$

derived from (2.3.)

To investigate the uniqueness we note that the equality

$$\frac{\partial \psi}{\partial x}\frac{dx}{d\nu} = \frac{\partial \phi}{\partial \nu} + x + \nu \frac{dx}{d\nu}$$

shows that $x$, $\nu$ are related by

$$\frac{\partial \psi}{\partial x} = \nu$$

Now (H3) is equivalent to the hypothesis that $\nu(x)$ is a concave function of $x$ for $x<-m$, or to the condition

$$\frac{\partial^3 E}{\partial x^3} = \frac{\partial^3 \psi}{\partial x^3} \leq 0$$

Since $E'(x)$ is concave and analytic, it is strictly concave and can therefore only vanish at one point in the region $x<-m$.

We next obtain an upper bound to $E(x)$ in the region $|x|>m_0$. If $|x|>m_0$ there exists $\nu \neq 0$ such that if

$$\rho_0^\Lambda = \exp[-\beta(H_0 - \nu M)]/\mathrm{tr}\exp[-\beta(H_0 - \nu M)]$$

then

$$\mathrm{tr}[\sigma_i \rho_0^\Lambda] = x^\Lambda \to x \tag{2.5}$$

as $|\Lambda| \to \infty$. We write

$$\varphi_0^\Lambda(i-j) = \langle(\sigma_i - \langle\sigma_i\rangle)(\sigma_j - \langle\sigma_j\rangle)\rangle$$

for the corresponding truncated two-point function.

(H4) For every $\nu \neq 0$ there exist a bound

$$\|\varphi_0^\Lambda\|_1 \leq C_0 < \infty$$

on the $L^1$ norm of the two-point function $\varphi_0^\Lambda$ uniformly as $|\Lambda| \to \infty$. That is the states $\rho_0^\Lambda$ are uniformly $L^1$-clustering.

**Theorem 3.** *If $|x|>m_0$ and $C_0$ is defined as in* (H4) *then*

$$E(x) \leq \psi_0(x) - \mu x + \alpha C_0 \|w\|_\infty \tag{2.6}$$

*Proof.* We see by (1.6) that

$$E^\Lambda(x^\Lambda) \le |\Lambda|^{-1}\{\mathrm{tr}\,[(H_0-\mu M)\rho_0^\Lambda]-\beta^{-1}\mathcal{S}(\rho_0^\Lambda)+\alpha\mathcal{W}(\rho_0^\Lambda)\}$$
$$= \psi_0^\Lambda(x^\Lambda)-\mu x^\Lambda+|\Lambda|^{-1}\alpha\mathcal{W}(\rho_0^\Lambda)$$
$$= \psi_0^\Lambda(x^\Lambda)-\mu x^\Lambda+\alpha\sum_{i\in\Lambda} w_p(i)\varphi_0^\Lambda(i)$$
$$\le \psi_0^\Lambda(x^\Lambda)-\mu x^\Lambda+\alpha C_0\|w_p\|_\infty$$

We note that $\|w_p\|_\infty \le \|w\|_\infty+\sum_{j\in Z^d\setminus\Lambda} w(j)$. Letting $|\Lambda|\to\infty$ we obtain (2.6) by using (2.5) and the locally uniform convergence of the thermodynamic functions.

We shall see in Section 4 that it is possible to choose $w$ in such a way that

$$\|w\|_\infty = o(\mu)$$

as $\mu\to 0$, which leads to the upper bound

$$E(x)\le\psi_0(x)-\mu x+o(\mu)$$

for $|x|>m_0$. While this is not valid if $|x|<m_0$ one can obtain other useful upper bounds by a similar method. Namely, one repeats the argument for a Gibbs state $\rho_0^\Lambda$ of the same type but at an inverse temperature $\beta(x)$ chosen so that $|x|$ is greater than the spontaneous magnetization. This ensures that the relevant two-point function is still clustering.

The above theorem provides us with a point $x<-m$ at which $E'(x)=0$. Since $E$ is strictly convex at this point, by analyticity, there exists a sequence $x(\Lambda)\to x$ such that

$$E^\Lambda(x(\Lambda))\to E(x),\qquad \frac{\partial}{\partial y}E^\Lambda\Big|_{y=x(\Lambda)}=0$$

According to the general theory we define the finite volume metastable states as

$$\tilde\rho^\Lambda=\exp[-\beta(H_0-\lambda M+\alpha V_{x(\Lambda)})]/\mathrm{tr}\exp[-\beta(H_0-\lambda M+\alpha V_{x(\Lambda)})]$$

with $\lambda$ determined by $|\Lambda|^{-1}\,\mathrm{tr}\,[M\tilde\rho^\Lambda]=x(\Lambda)$. Using (1.4) we can write equivalently

$$\tilde\rho^\Lambda=\exp[-\beta(H-\nu(\Lambda)M)]/\mathrm{tr}\exp[-\beta(H-\nu(\Lambda)M)]$$

with $\nu(\Lambda)$ given by

$$\frac{\partial\phi^\Lambda}{\partial\nu}\Big|_{\nu=\nu(\Lambda)}=-x(\Lambda).$$

By the Lemma 1(iv) we have the relation

$$\frac{\partial\phi^\Lambda}{\partial\nu}\Big|_{\nu=\mu+2\alpha x(\Lambda)}=-x(\Lambda),$$

that is

$$\nu(\Lambda)=\mu+2\alpha x(\Lambda)$$

We shall however adopt a definition which is slightly more convenient and equivalent in the thermodynamic limit, namely

$$\begin{aligned}\rho^\Lambda &= \exp[-\beta(H-\nu M)]/\mathrm{tr}\exp[-\beta(H-\nu M)] \\ &= \exp[-\beta(H_0-\mu M+\alpha V_x)]/\mathrm{tr}\exp[-\beta(H_0-\mu M+\alpha V_x)]\end{aligned} \tag{2.7}$$

where $x$ is determined by $E'(x)=0$, and $\nu=\mu+2\alpha x$. $\nu$ is called the effective field: it is always strictly negative since $x<-m$ implies that $\nu<\mu-2\alpha m<0$ by (2.4). Moreover we have

$$\mathrm{tr}[\sigma_i\rho^\Lambda] = -\frac{\partial\phi^\Lambda}{\partial\nu}(\nu) \to -\frac{\partial\phi}{\partial\nu}\bigg|_{\nu=\mu+2\alpha x} = x \tag{2.8}$$

as $|\Lambda|\to\infty$.

The following picture emerges from this analysis: the ensemble (2.7) which should describe the static properties of a metastable state for the system $H_0$ in a small positive magnetic field $\mu$ is given by a Gibbs ensemble associated with the perturbed system $H_0+\alpha V$ in a negative effective field $\nu$.

In the metastable state, only one thermodynamic phase should be present. This leads us to formulate a last hypothesis concerning the clustering properties of $\rho^\Lambda$:

(H5) Let $\varphi^\Lambda$ denote the truncated two-point function of the Gibbs state $\rho^\Lambda$ with respect to the Hamiltonian $H$ in the external field $\nu\neq 0$. Then there exists a bound

$$\|\varphi^\Lambda\|_1 \le C < \infty$$

uniformly as $|\Lambda|\to\infty$.

## 3. Dynamics

We now study the evolution of the metastable states $\rho^\Lambda$ just defined. Our goal is to prove that under a suitable stochastic dynamics the states have very long lifetimes for small $\mu>0$. Our calculations are adaptations of those of Penrose and Lebowitz [1, 2].

We start by developing the notation in a rather abstract form. We denote typical elements of the configuration space $2^\Lambda$ over the finite region $\Lambda$ by $\omega$, $\omega'$, .... The spin functions $\sigma_i$ are then maps from $2^\Lambda$ into $\{-1, 1\}$. We take the Gibbs state g to have the probability density

$$g(\omega) = \exp[-\beta(H_0-\mu M)(\omega)]/\sum_{\omega'}\exp[-\beta(H_0-\mu M)(\omega')]$$

so that

$$g(\omega)>0, \qquad \sum_\omega g(\omega)=1$$

A general Markov chain on the configuration space is given by the differential equations

$$\frac{\partial}{\partial t}p_t(\omega) = \sum_{\omega'} W_{\omega\omega'}p_t(\omega')$$

where

$$W_{\omega\omega'} \geq 0 \quad \text{if} \quad \omega \neq \omega'$$
$$W_{\omega\omega} \leq 0$$
$$\sum_{\omega} W_{\omega\omega'} = 0 \quad \text{for all} \quad \omega' \in 2^{\Lambda}.$$

The chain is said to satisfy the detailed balance condition with respect to $g$ if

$$W_{\omega\omega'} g(\omega') = W_{\omega'\omega} g(\omega) \tag{3.1}$$

for all $\omega$, $\omega'$. Putting

$$G_{\omega\omega'} = \delta_{\omega\omega'} g(\omega)$$

so that $G$ is a positive self-adjoint operator on $l^2(2^{\Lambda})$, the detailed balance condition may be rewritten in the operator form

$$WG = GW^*$$

or

$$G^{-1}WG = W^*.$$

If

$$X = G^{-1/2} W G^{1/2}$$

then $X$ is self-adjoint so $\mathrm{Sp}\,(X) \subseteq \mathbf{R}$. But the spectrum of $X$ coincides with that of $W$, and the fact that $W$ is the generator of a Markov chain implies that

$$\mathrm{Sp}\,(W) \subseteq \{z : \mathrm{Re}\, z \leq 0\}.$$

Therefore

$$\mathrm{Sp}\,(X) = \mathrm{Sp}\,(W) \subseteq \{x \in \mathbf{R} : x \leq 0\}.$$

Let $x_n \leq 0$ denote the eigenvalues of $X$ in decreasing order, and suppose that the Markov chain is erogdic, so that $x_0 = 0$ has multiplicity equal to one. Now let the metastable states $p$ have density

$$p(\omega) = aK(\omega) g(\omega)$$

where

$$0 < K(\omega) = \exp\,[-\beta\alpha V_x(\omega)] \leq 1 \tag{3.2}$$

and

$$a^{-1} = \sum_{\omega} K(\omega) g(\omega).$$

We wish to estimate the rate of return to equilibrium of $p_t = \exp\,(Wt)p$. Note that the assumptions of ergodicity implies that

$$\lim_{t\to\infty} p_t = g. \tag{3.3}$$

We shall estimate the rate of decay of $p_t$ using the function

$$f(t)=\langle p_t, aK\rangle$$

which would reduce to the function used by Penrose and Lebowitz [1, 6] if $K$ were the characteristic function of the set of permitted configurations in $2^\Lambda$.

**Lemma 4.** *The function* $f(t)$ *satisfies*

$$f(0)\exp[tf'(0)/f(0)]\le f(t)\le f(0)$$

*for all* $t\ge 0$.

*Proof.* By using the spectral theorem for $X$ we see that

$$\begin{aligned} f(t) &= \langle \exp(Wt)p, aK\rangle \\ &= \langle G^{1/2}\exp(Xt)G^{-1/2}p, aK\rangle \\ &= \langle \exp(Xt)(G^{-1/2}p), (G^{-1/2}p)\rangle \\ &= \sum_{n=0}^{\infty} \exp(x_n t) b_n \end{aligned}$$

where $b_n\ge 0$. This implies that $f(t)$ is logarithmically convex and monotonically decreasing, so

$$f(t)=\exp(q(t))$$

where

$$q(0)+tq'(0)\le q(t)\le q(0).$$

Hence

$$f(t)\ge f(0)\exp(tq'(0))=f(0)\exp[tf'(0)/f(0)].$$

This lemma allows one as in [1] to identify

$$R^\Lambda=-f'(0)/f(0) \tag{3.4}$$

as the decay rate of the system. To show that the metastable state $p$ takes a long time to relax to the Gibbs state $g$ one needs to show both that $R^\Lambda$ is small and that $f(\infty)/f(0)$ is small.

**Lemma 5.** *If* (H4) *and* (H5) *hold them.*

$$\lim_{|\Lambda|\to\infty}\{f(\infty)/f(0)\}=0.$$

*Proof.* Eq. (3.3) implies that

$$f(\infty)=\langle g, aK\rangle=1.$$

If $k(s)$ is defined by

$$\exp(k(s))=\sum_\omega a^s K^s(\omega)g(\omega)$$

then $k(s)$ is convex and $k(0)=k(1)=0$. Since

$$f(0)=\langle p, aK\rangle=\langle a^2K^2g, 1\rangle=\exp(k(2))$$

we have to show that

$$\lim_{|\Lambda|\to\infty} k(2)=+\infty$$

which follows from

$$\lim_{|\Lambda|\to\infty} k(\tfrac{1}{2})=-\infty.$$

Since

$$\exp(k(\tfrac{1}{2}))=\sum_\omega a^{1/2}K^{1/2}(\omega)g(\omega)=\langle p^{1/2}, g^{1/2}\rangle$$

and

$$\sum_\omega p(\omega)=\sum_\omega g(\omega)=1$$

this amounts to showing that the supports of $p$ and $g$ become essentially disjoint as $|\Lambda|\to\infty$. To establish this we define

$$2^\Lambda_+=\{\omega\in 2^\Lambda : \sum_i \sigma_i(\omega)\geq 0\}$$

and

$$2^\Lambda_-=2^\Lambda\setminus 2^\Lambda_+.$$

The clustering hypothesis (H4) and the assumption $\mu>0$ imply that

$$a^\Lambda_+=\sum_{\omega\in 2^\Lambda_-} g(\omega)$$

converges to zero as $|\Lambda|\to\infty$. Similarly the clustering hypothesis (H5) with $\nu<0$ imply that

$$a^\Lambda_+=\sum_{\omega\in 2^\Lambda_+} p(\omega)$$

converges to zero as $|\Lambda|\to\infty$. Therefore

$$\sum_{\omega\in 2^\Lambda} g(\omega)^{1/2}p(\omega)^{1/2}$$
$$\leq\Big[\sum_{,\omega\in 2^\Lambda_-} g(\omega)\Big]^{1/2}\cdot\Big[\sum_{\omega\in 2^\Lambda_-} p(\omega)\Big]^{1/2}+\Big[\sum_{\omega\in 2^\Lambda_+} g(\omega)\Big]^{1/2}\cdot\Big[\sum_{\omega\in 2^\Lambda_+} p(\omega)\Big]^{1/2}$$
$$\leq(a^\Lambda_+)^{1/2}+(a^\Lambda_-)^{1/2}$$

which converges to zero as $|\Lambda|\to\infty$, as required.

We now return to the analysis of $R^\Lambda$, defined in (3.4). If we write $\omega\sim\omega'$

when $\sigma_i(\omega)=\sigma_i(\omega')$ for all except one site $i\in\Lambda$, then the Glauber stochastic dynamics is obtained by putting

$$W_{\omega\omega'}=g(\omega)^{1/2}g(\omega')^{-1/2}$$

if $\omega\sim\omega'$,

$$W_{\omega'\omega'}=-\sum_{\omega\sim\omega'}W_{\omega\omega'}$$

and $W_{\omega\omega'}=0$ for all other pairs $\omega,\omega'$. The detailed balance condition (3.1) and ergodicity are readily verified.

**Lemma 6.** *We have*

$$R^{\Lambda}\leq\beta\alpha\exp[\beta(\mu+2\,\|h\|_1+8\alpha)]\langle Y\rangle_{\rho'} \tag{3.5}$$

*where*

$$Y(\omega)=\sum_{\omega'\sim\omega}|V_x(\omega)-V_x(\omega')|$$

*and $\rho'$ is the Gibbs state with respect to the Hamiltonian*

$$H_0-\mu M+2\alpha V_x. \tag{3.6}$$

*Proof.* We start with the estimate

$$\begin{aligned}-f'(0)&=-a^2\langle WKg,K\rangle\\&=-a^2\sum_{\omega'\omega}W_{\omega\omega'}K(\omega)K(\omega')g(\omega')\\&=-a^2\sum_{\omega\sim\omega'}W_{\omega\omega'}K(\omega)K(\omega')g(\omega')+a^2\sum_{\omega\sim\omega'}W_{\omega\omega'}K(\omega')^2g(\omega')\\&\leq a^2\sum_{\omega\sim\omega'}W_{\omega\omega'}K(\omega')g(\omega')\,|K(\omega)-K(\omega')|\\&=a^2\sum_{\omega\sim\omega'}K(\omega')g(\omega)^{1/2}g(\omega')^{1/2}\,|K(\omega)-K(\omega')|\\&\leq a^2\beta\alpha\sum_{\omega\sim\omega'}K(\omega')g(\omega)^{1/2}g(\omega')^{1/2}\max\{K(\omega),K(\omega')\}\,|V_x(\omega)-V_x(\omega')|\end{aligned}$$

by (3.2). Now since $\omega$ is obtained from $\omega'$ by reversing the sign of only one spin, we have

$$\begin{aligned}&|\log g(\omega)-\log g(\omega')|\\&\quad=\beta\,|(H_0-\mu M)(\omega)-(H_0-\mu M)(\omega')|\\&\quad\leq 2\beta(\mu+2\,\|h\|_1).\end{aligned}$$

Therefore

$$g(\omega)^{1/2}\leq g(\omega')^{1/2}\exp[\beta(\mu+2\,\|h\|_1)].$$

Similarly

$$\begin{aligned}
&|\log K(\omega)-\log K(\omega')| \\
&\quad =\beta\alpha\,|V_x(\omega)-V_x(\omega')| \\
&\quad =\beta\alpha\,|V(\omega)-2xM(\omega)-V(\omega')+2xM(\omega')| \\
&\quad \leq \beta\alpha\,|4\,\|w\|_1+4\,|x|| \\
&\quad \leq 8\beta\alpha
\end{aligned}$$

so

$$\max\{K(\omega),K(\omega')\}\leq K(\omega')\exp(8\beta\alpha).$$

We deduce that

$$-f'(0)\leq a^2\beta\alpha\exp[\beta(\mu+2\,\|h\|_1+8\alpha)]\sum_{\omega\sim\omega'}K(\omega')^2g(\omega')\,|V_x(\omega)-V_x(\omega')|$$

which leads quickly to (3.5). The presence of the factor 2 in (3.6) is surprising, and is a nuisance because it prevents one from using (2.8), but the factor is removed in the next lemma.

**Lemma 7.** *If $\rho^\Lambda$ is the Gibbs state with respect to the Hamiltonian*

$$H_0-\mu M+\alpha V_x$$

then

$$\langle Y\rangle_{\rho'}\leq 4w_p(0)\,|\Lambda|+4\langle V_x\rangle_{\rho^\Lambda}^{1/2}\,|\Lambda|^{1/2}.$$

*Proof.* If $V_x^{(r)}$ is obtained from $V_x$ by reversing the sign of the spin at the site $r$ then we deduce from (1.4) that

$$\begin{aligned}
|V_x-V_x^{(r)}| &= |-4w_p(0)\sigma_r x+2\sum_{\substack{i\neq r\\ i\in\Lambda}}w_p(i-r)(\sigma_i-x)2\sigma_r| \\
&= |-4w_p(0)+4\sum_{i\in\Lambda}w_p(i-r)(\sigma_i-x)\sigma_r| \\
&\leq 4w_p(0)+4A_r
\end{aligned}$$

where

$$A_r=\left|\sum_{i\in\Lambda}w_p(i-r)(\sigma_i-x)\right|.$$

Therefore

$$\begin{aligned}
\langle Y\rangle_{\rho'} &= \sum_{r\in\Lambda}\langle|V_x-V_x^{(r)}|\rangle_{\rho'} \\
&\leq 4w_p(0)\,|\Lambda|+4\sum_{r\in\Lambda}\langle A_r\rangle_{\rho'} \\
&\leq 4w_p(0)|\Lambda|+4\left\langle\sum_{r\in\Lambda}A_r^2\right\rangle^{1/2}|\Lambda|^{1/2}.
\end{aligned}$$

Next observe that

$$\sum_{r\in\Lambda} A_r^2 = \sum_{i,j\in\Lambda}\sum_{r\in\Lambda} w_p(i-r)w_p(j-r)(\sigma_i - x)(\sigma_j - x)$$
$$= \sum_{i,j\in\Lambda} V_p(i-j)(\sigma_i - x)(\sigma_j - x)$$

Since the Fourier transform of $V_p(i)$ on $\Lambda$ satisfies

$$0 \le \hat{V}_p(k) = (\hat{w}_p(k))^2 \le \hat{w}_p(k)$$

for all $k \in Z^d$ one gets

$$0 \le \left\langle \sum_{r\in\Lambda} A_r^2 \right\rangle \le \langle V_x \rangle_{\rho'}$$

The proof is completed by using the monotonicity of the function

$$\lambda \to \operatorname{tr}[V_x \exp[-\beta(H_0 - \mu M + \lambda V_x)]]/\operatorname{tr}\exp[-\beta(H_0 - \mu M + \lambda V_x)]$$

to replace the expectation with respect to $\rho'$ by that with respect to $\rho^\Lambda$.

The droplet model of condensation predicts that the decay rate is proportional to the volume, and so indicates that in the thermodynamic limit one should define the decay rate per unit volume by

$$R^\infty = \limsup_{|\Lambda|\to\infty} (R^\Lambda/|\Lambda|)$$

**Theorem 8.** *Under the hypotheses* (H1) *to* (H5), *one has*

$$R^\infty \le 4\beta\alpha \exp[\beta(\mu + 2\|h\|_1 + 8\alpha)]\, \|w\|_\infty^{1/2}(1 + C^{1/2}) \tag{3.7}$$

*Proof.* Putting

$$x^\Lambda = \operatorname{tr}(\sigma_i \rho^\Lambda)$$

we see that

$$\langle V_x \rangle_{\rho^\Lambda} = \sum_{i,j\in\Lambda} w(i-j)\langle(\sigma_i - x)(\sigma_j - x)\rangle_{\rho^\Lambda}$$
$$= \sum_{i,j\in\Lambda} w(i-j)\langle(\sigma_i - x^\Lambda)(\sigma_j - x^\Lambda)\rangle_{\rho^\Lambda} + |\Lambda|(x^\Lambda - x)^2$$
$$\le |\Lambda|\,\{\|w\|_\infty \|\varphi^\Lambda\|_1 + (x^\Lambda - x)^2\}$$

so

$$R^\Lambda \le \beta\alpha \exp[\beta(\mu + 2\|h\|_1 + 8\alpha)][4w(0)\,|\Lambda| + 4(\|w\|_\infty \|\varphi^\Lambda\|_1 + (x^\Lambda - x)^2)^{1/2}\,|\Lambda|^{1/2}]$$

By (2.8) and (H5) we deduce that

$$R^\infty \le 4\beta\alpha \exp[\beta(\mu + 2\|h\|_1 + 8\alpha)][4w(0) + 4(\|w\|_\infty C)^{1/2}]$$
$$\le 4\beta\alpha \exp[\beta(\mu + 2\|h\|_1 + 8\alpha)]\, \|w\|_\infty^{1/2}(1 + C^{1/2}).$$

One sees from (3.7) that the decay rate $R^\infty$ is small if the strength $\alpha$ of the constraint $\mathcal{W}$ is small, and also $\|w\|_\infty$ is small. This second condition is closely related to the assumption that the range $\gamma$ of $w$ is large, as we shall see in Section 4, where our bound on $R^\infty$ is compared with that in [6].

## 4. Discussion

It is clear that the precise form of our metastable states depends on the choice of $w$ and $\alpha$, and we do not have a general principle leading to a single canonical choice. However, for each small value of the external field $\mu > 0$, $w$ and $\alpha$ should be fixed so that the ensemble (2.7) has the physical properties of a metastable state: its life time should be long and its magnetization $x(\mu) < 0$ should provide a smooth continuation of the negative part of the magnetization curve of $H_0$.

It is likely that the main important feature of $w$ is its range

$$\gamma = \sum_i |i| \, w(i)$$

giving the scale on which magnetization fluctuations are suppressed. $\gamma$ should be of the same order of magnitude as the critical droplet size in the droplet model of condensation namely $\gamma = O(\mu^{-1})$.

To simplify the discussion, we suppose that we are given a single one-parameter family $w_\gamma$ of the form

$$w_\gamma(i) = \gamma^{-d} f(i/\gamma) \Big/ \sum_j \gamma^{-d} f(j/\gamma)$$

$f$ is a fixed integrable function of positive type, such as $f(x) = \exp(-x^2)$, so that $w_\gamma$ fulfill the requirements of Section I. The denominator has a finite non-zero limit as $\gamma \to \infty$, therefore one has

$$\|w_\gamma\|_\infty \leq b^2 \gamma^{-d} \tag{4.1}$$

With such a choice of $w_\gamma$ all the quantities in the last section depend upon the two real parameters $\alpha$, $\gamma$ and from now on, we shall discuss them as functions of $\alpha$, $\gamma$ instead of functionals of $\alpha$ and general $w$. In particular we have the two parameter family of systems $H(\alpha, \gamma)$ with spontaneous magnetization $m(\alpha, \gamma)$.

According to (2.4) a sufficient condition for the existence of a metastable state $\rho^\Lambda(\alpha, \gamma)$ in the external field $\mu > 0$ is the inequality

$$2\alpha m(\alpha, \gamma) > \mu \tag{4.2}$$

This defines a permitted region for metastable states in the parameter space $\alpha$, $\gamma$ for given $\mu > 0$. Notice that according to (H1) this region is contained in the half-space $\alpha > \mu/2m_0$. In order to get a qualitative view of its shape, let us make the following model for the function $m(\alpha, \gamma)$:

$$m(\alpha, \gamma) = m_0 - m_1 \alpha\gamma, \qquad m_1 > 0 \tag{4.3}$$

This choice is suggested by the rough idea that $\alpha V$ being an antiferromagnetic perturbation of $H_0$, the spontaneous magnetization of $H(\alpha, \gamma)$ should decrease when both the strength and the range of the perturbation are increased, and $m(0, \gamma) = m(\alpha, 0) = m_0$.

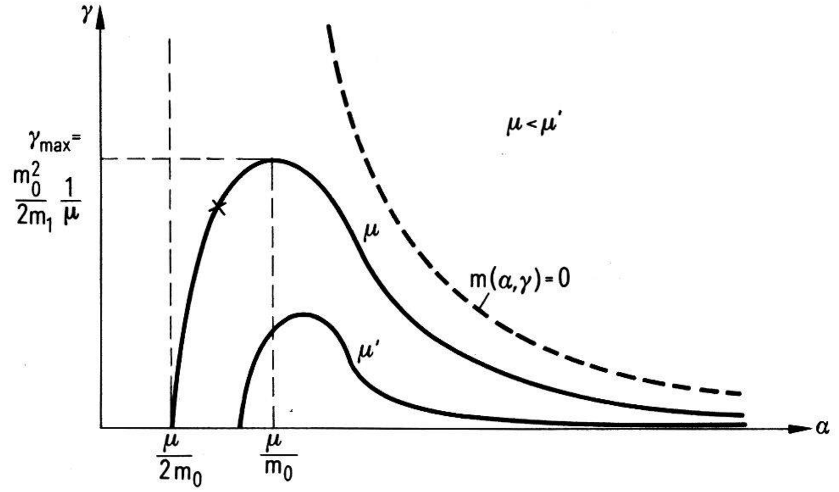


Figure 2
The region below the solid curve is the permitted region of parameters $\alpha$, $\gamma$ in the external field $\mu > 0$.

For $\alpha$, $\gamma$ satisfying (4.2), one can estimate the life time of the metastable state $\rho^\Lambda$ by the procedure of Section 3. One sees that in the formula (3.7), the constant $C$ obtained from (H5) may depend on $\alpha$, $\gamma$, $\mu$ through the state $\rho^\Lambda$. Remembering that $\phi^\Lambda$ is the truncated two point function associated with the Hamiltonian $H(\alpha, \gamma)$ in the effective field $\nu < 0$, it is plausible that the $L^1$-fluctuations $\|\varphi^\Lambda\|_1$ are uniformly bounded provided that one keeps away from the values of $\alpha$, $\gamma$ for which the temperature $\beta^{-1}$ is critical for $H(\alpha, \gamma)$. In other words, $\|\varphi^\Lambda\|_1$ should be finite whenever $m(\alpha, \gamma) \neq 0$. We assume this in the following strong form

(H6) There exist constants $k$, $n$ such that if $2\alpha m > \mu$ and $\nu \neq 0$ then

$$\|\varphi^\Lambda\|_1 \leq k^2 m^{-n}$$

for all large enough $\Lambda$.

Using this hypothesis and (4.1), we obtain from Theorem 8 that

$$R^\infty \leq 4\beta\alpha b\gamma^{-d/2} \exp\left[\beta(\mu + 2\|h\|_1 + 8\alpha)\right](1 + km(\alpha, \gamma)^{-n/2}) \tag{4.4}$$

If $\alpha \leq \mu/m_0$, we have $m(\alpha, \gamma) \geq m_0/2$ and $R^\infty = O(\alpha\gamma^{-d/2})$. This shows that we will obtain a small value for the bound (4.4) if we choose $\alpha$, $\gamma$ on the part of the boundary of the permitted region with $\alpha \leq \mu/m_0$. (Such a choice is marked * on the figure.)

When $\alpha$, $\gamma$ are chosen on the boundary i.e. $2\alpha m(\alpha, \gamma) = \mu$, $E(x)$ does not have a local minimum when $x < -m$, but just a turning point at $x = -m$. The corresponding metastable state is then not the Gibbs state with respect to $H$ in the effective field $\nu < 0$, but the Gibbs state with zero effective field and with negative boundary conditions. In this case, the magnetization of the metastable state is simply given by

$$x(\mu) = -m(\alpha, \gamma) = -\mu/2\alpha.$$

Then one can choose functions $\alpha(\mu)$, $\gamma(\mu)$ such that

$$\lim_{\mu\to 0} \alpha(\mu) = 0, \qquad \lim_{\mu\to 0} \gamma(\mu) = +\infty$$

$$\lim_{\mu\to 0} m(\mu) = \lim_{\mu\to 0} m(\alpha(\mu), \gamma(\mu)) = m_0$$

and

$$R^{\infty} = O(\alpha(\mu)\gamma(\mu)^{-d/2}).$$

We can set for instance $\alpha(\mu) = \mu/2m_0 + O(\mu^{1+\varepsilon})$ then

$$\gamma(\mu) = O(\mu^{-(1-\varepsilon)}), \qquad m(\mu) = m_0 + O(\mu^{\varepsilon})$$

and

$$R^{\infty} = O(\mu^{1+d/2-\varepsilon d/2}). \tag{4.5}$$

We remark that the largest possible range $\gamma$ (corresponding to the smallest decay rate) is obtained when $\varepsilon = 0$, namely $\gamma = O(\mu^{-1})$.

This discussion indicates that it should be possible to define a sequence of metastable states with continuous magnetization curve and vanishing decay rate per unit volume as $\mu \to 0$. The discussion is based on the admittedly heuristic form (4.3) of the function $m(\alpha, \gamma)$, but we hope that it is at least qualitatively correct.

The form of the continuation of the magnetization curve in the metastable region and the possible existence of a coercive field merit further investigation. (Notice that any continuation will satisfy $m(\mu) < m_0$ by (H1).) In our setting information on these questions could be obtained by getting more insight into the properties of the family $H(\alpha, \gamma)$. More generally, it would be interesting to study in more detail the problem of perturbation of ferromagnetic systems and prove various hypothesis given in the text.

The reader may have noticed that while the method of Lagrange multipliers instructs one to look for stationary points of $\mathscr{E}(\rho)$, we have in fact only looked for local minima. While the intuitive reason for this seems clear, the mathematical justifications are less obvious. We investigate this extra condition in the very general context discussed at the beginning of Section 2.

Let $\rho_\alpha \in X$ be at a local minimum of $\mathscr{E}_\alpha = \mathscr{F} + \alpha\mathscr{W}$, and suppose that all functions are differentiable with respect to $\alpha$. Then

$$\begin{aligned} 0 &= \mathscr{E}'(\rho_\alpha) = \mathscr{F}'(\rho_\alpha) + \alpha\mathscr{W}'(\rho_\alpha) \\ 0 &\le \mathscr{E}''(\rho_\alpha) = \mathscr{F}''(\rho_\alpha) + \alpha\mathscr{W}''(\rho_\alpha) \end{aligned} \tag{4.6}$$

where the derivatives are vectors or matrices. Differentiating (4.6) we obtain

$$0 = \mathscr{F}''(\rho_\alpha)\rho'_\alpha + \mathscr{W}'(\rho_\alpha) + \alpha\mathscr{W}''(\rho_\alpha)\rho'_\alpha$$

so

$$\begin{aligned} 0 &\le \langle(\mathscr{F}''(\rho_\alpha) + \alpha\mathscr{W}''(\rho_\alpha))\rho'_\alpha, \rho'_\alpha\rangle \\ &= -\langle\mathscr{W}'(\rho_\alpha), \rho'_\alpha\rangle \\ &= -\frac{\partial}{\partial\alpha}\mathscr{W}(\rho_\alpha) \end{aligned}$$

and $\mathcal{W}(\rho_\alpha)$ is a monotonically decreasing function of $\alpha$. In other words, if one weakens the constraint by reducing $\alpha$, one obtains a metastable state with larger fluctuations. This process does not continue indefinitely, however, because if $\alpha$ is too small one obtains

$$2\alpha m(\alpha, \gamma) < \mu$$

and there is no metastable state. The criterion of minimum constraint suggests that one should let $\alpha$ be the smallest value for which a metastable state exists, and this leads once again to the equation

$$2\alpha m(\alpha, \gamma) = \mu$$

We have not, however, found any principle for determining $\gamma$ apart from that of minimizing $R^\infty$.

We finally compare our results with those obtained in [6] for the nearest neighbour Ising model. With a technically different definition of metastability, which does not have the thermodynamic features of our definitions Capoccaccia et al [6] obtained a bound of the form

$$R^\infty = O(\exp(-b/\mu))$$

as $\mu \to 0$. The indications from (4.5) are that the best we can hope for is

$$R^\infty = O(\mu^{1+d/2})$$

which should also be compared with (5.2) of [4].

We believe that this is an intrinsic limitation of our approach in that we only attempt to control second order fluctuations. There is a sense in which the use of a restricted configuration space as in [1, 6] amounts to controlling $n$-th order correlations of all orders $n$, or equivalently to adding onto the Hamiltonian $H_0 - \mu M$ a potential $V$ which contains multi-body interactions of all orders. One would conjecture that for all finite $N$ there exists a definition of metastability in which one only controls correlations of order $\leq N$ and such that the decay rate is a decreasing function of $N$.

While one might claim that the "best" theory of metastability is the one leading to the slowest decay, this is by itself not a satisfactory criterion. the correct procedure is surely to devise a *dynamical* model for the formation of metastable states, by for example starting with a Gibbs state and then changing the thermodynamic parameters smoothly until the state becomes metastable. A dynamical definition of metastability has been considered and studied numerically in [7] (see references quoted in [7]). The relationship of such a purely dynamical approach to metastability to one of the above static definitions should then be investigated.

## 5. The van der Waals limit

In this section, we treat in our scheme the weak long range limit (Kac potential). In this limit, the thermodynamic functions introduced in Section 2 can be found explicitly and $E(x)$ determines the same metastable states as those of the usual van der Waals theory.

We consider first a special case in our setting in which the constraint $w$ is chosen proportional to the interaction $h$ (assuming here $h$ both positive and positive definite)

$$w(i) = h(i)/a, \qquad a = \|h\|_1. \tag{5.1}$$

Then $H(\alpha) = (1-\alpha/a)H_0$ becomes a one parameter family, the range $\gamma$ of $w$ being fixed and equal to that of the interaction. It follows from the definitions that $\psi(x)$ and $E(x)$ can be deduced directly from the knowledge of $\psi_0(x)$:

$$\psi(x, \beta) = (1-\alpha/a)\psi_0(x, \beta(1-\alpha/a)) \tag{5.2}$$

Moreover, for $\alpha < a$, $H(\alpha)$ is ferromagnetic with spontaneous magnetization given by

$$m(\alpha) = m_0(\beta(1-\alpha/a))$$

We have $m(\alpha) \leq m_0$ since $m_0(\beta)$ is a decreasing function of the temperature.

The weak long range limit is defined by choosing a family of interactions $h_\gamma(i) = \gamma^{-d}h(i/\gamma)$ with $\|h\|_1 < \infty$ and letting $\gamma \to \infty$ after the thermodynamic limit. It is well known [8] that the corresponding free energy density $\psi_0^\gamma(x)$ converges to

$$\psi_0(x) = \xrightarrow{\text{conv}} \Xi_0(x) \tag{5.3}$$

where $\xrightarrow{\text{conv}}$ means convex envelope. $\Xi_0$ is the usual mean field function

$$\Xi_0(x) = -ax^2 - \beta^{-1}S(x)$$

with

$$S(x) = -\left(\frac{1+x}{2}\right)\log\left(\frac{1+x}{2}\right) - \left(\frac{1-x}{2}\right)\log\left(\frac{1-x}{2}\right).$$

For $\beta a \leq 1$ one has $\psi_0(x) = \Xi_0(x)$ while for $\beta a > 1$, the functions $\psi_0(x)$ and $\Xi_0(x)$ coincide only for $|x| > m_0$. The spontaneous magnetization $m_0(\beta)$ is a monotonically increasing function of $\beta$ for $\beta a > 1$ given by the (positive) solution of

$$\frac{1+m_0}{1-m_0} = \exp(2a\beta m_0).$$

Since in the limit of infinitely long range interaction, we expect the critical droplet size in any external field $\mu$ to be also infinite, we are led to choose the constraint as in (5.1) with $w_\gamma(i) = h_\gamma(i)/a$. After the thermodynamic limit and letting $\gamma \to \infty$ we obtain therefore by (5.2) and (5.3)

$$\psi(x) = \xrightarrow{\text{conv}} \Xi(x)$$

with

$$\Xi(x) = -(a-\alpha)x^2 - \beta^{-1}S(x)$$

**Theorem 9.** *If* $\beta(a-\alpha) > 1$ *one has*

$$E(x) = \begin{cases} \Xi_0(x) - \mu x & |x| > m(\alpha) \\ \Xi_0(m(\alpha)) - \mu x - \alpha(x^2 - m(\alpha)^2) & |x| \leq m(\alpha) \end{cases}$$

*Proof.* For $|x|>m$, $\Xi(x)$ is convex and one has

$$\psi(x)=\Xi(x)=\Xi_0(x)+\alpha x^2$$

$$E(x)=\psi(x)-\mu x-\alpha x^2=\Xi_0(x)-\mu x$$

For $x\leq m$, $\psi(x)=\Xi(m)$ and one finds

$$E(x)=\Xi(m)-\mu x-\alpha x^2=\Xi_0(m)-\mu x-\alpha(x^2-m^2).$$

We see that for $\alpha>\mu/m(\alpha)$ the location of the relative minimum of $E(x)$ is the same as that of $\Xi_0-\mu x$, thus determining the same metastable state as in the mean field theory.

We leave the reader to compute further thermodynamic quantities and to study the dynamics according to the principles of Section 3. (In particular, $R^\infty=0$ for all $\mu$ since one can let $\gamma\to\infty$.)

Before concluding this section, let us note that there is another case which can be treated analytically, namely choosing for $H_0$ the 2-dimensional next neighbour Ising model and $w$ as in (5.1). $m(\alpha)=m_0(\beta(1-\alpha/a))$ is then given explicitly by the Onsager magnetization $m_0(\beta)$ and one can determine $\alpha(\mu)$ according to the same principle as in Section 4 by solving $2\alpha m(\alpha)=\mu$ for $\mu$ small enough. The corresponding metastable states in positive field are states of the Ising model with a reduced interaction strength and negative boundary conditions. These states are certainly not the best candidates to describe metastability since the range $\gamma$ of the constraint cannot be varied to maximize the life time.

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## 6. Appendix

We investigate the hypotheses (H1) to (H6) for two particular models which have been studied in some detail over the last fifteen years.

(n.n) $H_0$ is the two-dimensional nearest neighbour Ising model. That is

$$h(i-j)=\tfrac{1}{2}J>0$$

if $i$, $j$ are nearest neighbours and $h(i-j)$ vanishes otherwise. Because the Hamiltonian $H=H_0+\alpha V$ is not ferromagnetic this case must be studied using perturbation theory. We assume that $\beta>\beta_0$ throughout.

(f) We have $h=h_1+h_2$ where $h_1$ is the above nearest neighbour interaction and $h_2(i)>0$ for all $i$. Moreover $w$ is of compact support and $\alpha>0$ is small enough so that

$$0\leq\alpha w(i)\leq h_2(i) \tag{6.1}$$

for all $i$. This case is studied using ferromagnetic inequalities.

(H1) In the n.n. case, it follows from [9] or [10, p. 114] that the spontaneous magnetization $m(\alpha, \gamma)$ is strictly positive for $\alpha\gamma < K$. In the $f$ case, one obtains the strict positivity of $m(\alpha, \gamma)$ subject to (6.1) by applying the *GKS* inequalities. See [11, 12] or [10, p. 120].

(H2) Because

$$\psi(x) = \phi(\mu) + \mu x$$

where $x$ is determined by

$$\frac{\partial \phi}{\partial \mu} = -x$$

we see that

$$\frac{\partial \psi}{\partial x}\frac{dx}{d\mu} = \frac{\partial \phi}{\partial \mu} + x\frac{dx}{d\mu}$$

so that

$$\frac{\partial \psi}{\partial x} = \mu$$

Thus $\psi(x)$ is analytic for $|x| > m$ with $\psi'(\pm m) = 0$ if and only if $\phi(\mu)$ is analytic for $\mu \neq 0$.

For the $f$ case this is an immediate consequence of the Lee-Yang theorem [10, p. 110]. A corresponding result for the n.n. case has been obtained by Ruelle [13], who, however, gives no indication of the magnetitude of $\alpha$, $\gamma$ for which his results hold.

(H3) For the $f$ case this is a consequence of the *GHS* inequalities [14], a simple proof of which may be found in [15].

(H4–H6) Clustering properties as strong as those needed here have not been proved except for the n.n. Ising Hamiltonian in two dimensions [16]. We refer to [17, 18] and references cited there for clustering properties of ferromagnetic Hamiltonians. In the ferromagnetic case, the *GKS* inequalities imply that the infinite volume two-point functions satisfy

$$\varphi^{\infty}(i) = \langle \sigma_i \sigma_0 \rangle - \langle \sigma_i \rangle \langle \sigma_0 \rangle \geq 0$$

so

$$\|\varphi^{\infty}\|_1 = \sum_{i \in Z^d} (\langle \sigma_i \sigma_0 \rangle - \langle \sigma_i \rangle \langle \sigma_0 \rangle) = \frac{\partial m}{\partial \nu} = \chi(\nu) \tag{6.2}$$

where $\chi(\nu)$ is the susceptibility in the external field $\nu$.

For potentials decreasing as power laws, the general position seems to be that below the critical temperature and for fixed $\nu \neq 0$ the two point function decreases at infinity at the same rate as the potential, so that by (6.2), the susceptibility is finite. It is a simple consequence of the GHS inequalities that the susceptibility is a decreasing function of the external field $\nu$ when $\nu > 0$. As $\nu \to 0$ the susceptibility converges to the susceptibility for zero field with positive boundary conditions, which should also be finite. The zero field susceptibility should be uniformly bounded provided one keeps away from the values of $\alpha$, $\gamma$ for which $\beta$ equals the critical temperature. There is, however, no real evidence for the precise form of the divergence of $\chi(0+)$ as the critical temperature of the Hamiltonian $H(\alpha, \gamma)$ converges to $\beta$.

When one turns to finite volume correlation functions $\varphi^{\Lambda}$ one should have the same type of bounds for large enough $\Lambda$. However, one has to take into account the presence of the phase transition at zero field, by accepting that the rate of convergence of $\|\varphi^{\Lambda}\|_1$ as $|\Lambda| \to \infty$ is very slow for small $\nu \neq 0$.

## REFERENCES

[1] O. Penrose and J.-L. Lebowitz, *Rigorous Treatment of Metastable States in the van der Waals–Maxwell Theory.* J. Stat. Phys. *3* (1971) 211–236.
[2] O. Penrose and J.-L. Lebowitz, *Towards a rigorous molecular theory of metastability.* p. 293–340 of *Fluctuation Phenomena*, Studies in Stat. Mech. Vol. 7, eds. E. W. Montroll and J.-L. Lebowitz, North-Holland, 1979.
[3] E. B. Davies, *Symmetry breaking for a non-linear Schrödinger equation.* Commun. Math. Phys. *64* (1979), 191–210.
[4] E. B. Davies, *Metastable states of molecules.* Commun. Math. Phys. *75* (1980), 263–283.
[5] G. L. Sewell, *Stability, equilibrium and metastability in statistical mechanics*, Phys. Rep. *57* (1980), 307–342.
[6] D. Capocaccia, M. Cassandro and E. Olivieri, *A study of metastability in the Ising model.* Commun. Math. Phys. *39* (1974), 185–205.
[7] K. Binder and H. Müller-Krumbhaar, *Investigation of metastable states and nucleation in the kinetic Ising model.* Phys. Rev. *B9* (1974), 2328–2353.
[8] J.-L. Lebowitz and O. Penrose, *Rigorous Treatment of the van der Waals-Maxwell Theory of the Liquid-Vapor Transition.* J. Math. Phys. 7 (1966), 98–113.
[9] A. Ginibre, A. Grossman and D. Ruelle, *Condensation of lattice gases.* Commun. Math. Phys. *3* (1966), 187–195.
[10] D. Ruelle, *Statistical mechanics.* W. A. Benjamin Inc. 1969.
[11] R. B. Griffiths, *Correlations in Ising ferromagnets* (I). J. Math. Phys. *8* (1967), 478–483. (II). J. Math. Phys. *8* (1967), 484–489.
[12] D. G. Kelly and S. Sherman, *General Griffiths inequalities in Ising ferromagnets.* J. Math. Phys. *9* (1968), 466–484.
[13] D. Ruelle, *Some remarks on the location of zeros of the partition function for lattice systems.* Commun. Math. Phys. *31* (1973), 265–277.
[14] R. B. Griffiths, C. A. Hurst and S. Sherman, *Concavity of magnetization of an Ising ferromagnet in a positive external field.* J. Math. Phys. *11* (1970), 790–795.
[15] J.-L. Lebowitz, *GHS and other inequalities*, Commun. Math. Phys. *35* (1974), 87–92.
[16] A. Martin-Löf, *Mixing properties, differentiability of the free energy and the central limit theorem for a pure phase in the Ising model at low temperature.* Commun. Math. Phys. *32* (1973), 75–92.
[17] M. Duneau, B. Souillard and D. Iagolnitzer, *Decay of correlations for infinite range interactions.* J. Math. Phys. *16* (1975), 1662–1666.
[18] D. Iagolnitzer and B. Souillard, *Decay of correlations for slowly decreasing potentials.* Phys. Rev. *A16* (1977), 1700–1704.
[19] E. B. Davies, *Metastable states of symmetric Markov semigroups.* In preparation.

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