Journal of Statistical Physics, Vol. 27, No. 4, 1982

Metastability and the Ising Model

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Received May 13, 1981; revised September 22, 1981

We discuss a recent theorem which establishes a precise connection between (i) the approximate degeneracy of the zero eigenvalue for the generator of the Glauber dynamics of the Ising model in a small nonzero field and below the critical temperature, (ii) the existence of a partition of the configuration space into a normal region and a metastable region. This enables us to demonstrate that the recent approach to metastability of Davies and Martin may be viewed as a simple (although in some ways fairly crude) approximation to the conventional approach. We also obtain what appear to be the first results concerning the stability of metastable states under small perturbations.

KEY WORDS: Metastability; Ising model; Glauber dynamics.

1. INTRODUCTION

In an earlier paper,[7] Ph. A. Martin and the author described a new approach to metastability for classical lattice systems, which grew out of analogous work on small quantum systems.[3–5] The author subsequently[6] carried out a systematic and purely mathematical investigation of metastability for symmetric Markov semigroups, which established a strong connection between approximate degeneracy of the ground state of the system and the existence of a metastable region in the configuration space. The goal of the present paper is to draw these various ideas together and to discuss their physical implications. Our work is a contribution to the very sparse mathematically rigorous literature on metastability of classical systems, which is excellently surveyed by Penrose and Lebowitz[8] and Sewell.[10]

For the sake of definiteness we shall confine attention throughout to the nearest neighbor Ising model in $d \geqslant 2$ dimensions, although reference

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0022-4715/82/0400-0657$03.00/0

to Refs. 6 and 7 will make it clear that our ideas have a much wider scope. We start with a region

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

of volume $|\Lambda| = N^d$ and with periodic boundary conditions. The configuration space of the system is then 2^Λ. At each site $i \in \Lambda$ one has a spin $\sigma_i = \pm 1$, and the finite-volume Hamiltonian is defined at $\omega \in 2^\Lambda$ by

$$\mathcal{H}_0(\omega) = J \sum_{i \sim j} \sigma_i \sigma_j$$

where $i \sim j$ signifies that i and j are nearest neighbors. We also put

$$\mathfrak{M}(\omega) = \sum_i \sigma_i$$

and suppose that the temperature β^{-1} of the system is significantly smaller than the critical temperature β_c^{-1} for the phase transition. The Gibbs state of the system in the external field $\mu > 0$ assigns the probability

$$g(\omega) = \frac{\exp\{-\beta[\mathcal{H}_0(\omega) - \mu\mathfrak{M}(\omega)]\}}{\sum_{\omega'} \exp\{-\beta[\mathcal{H}_0(\omega') - \mu\mathfrak{M}(\omega')]\}} \tag{1.1}$$

to the site $\omega \in 2^\Lambda$.

We emphasized in Ref. 7 that we were only interested in studying translation-invariant states, a restriction which might be important in $d > 2$ dimensions. This can be accomplished within the notation of Ref. 6 by defining X to be the set of orbits in 2^Λ under the action of the translation group. If $\theta : 2^\Lambda \to X$ is the natural map which assigns each point to its orbit, we define an integral on X by putting

$$\int_X f(x)\,dx = \sum_{\omega \in 2^\Lambda} f(\theta(\omega)) g(\omega)$$

for all $f : X \to \mathbb{C}$. The volume (or probability) of a set E in X is defined by

$$|E| = \int_E dx = \int_X \chi_E(x)\,dx$$

It is clear that $|X| = 1$, so that X is a probability space. Since X is finite the spaces $L^p(X)$ are equal for $1 \leqslant p \leqslant \infty$, and we shall often write $L(X)$ for them all, but still distinguish between the different L^p norms $\|\cdot\|_p$.

We define the inner product of $f, h \in L^2(X)$ by

$$\langle f, h \rangle = \int_X f(x)\overline{h(x)}\,dx$$

We also define the map $T : L^1(X) \to l^1(2^\Lambda)$ by

$$(Tf)(\omega) = f(\theta\omega)\, g(\omega) \tag{1.2}$$

It is easy to check that T is isometric for the L^1 norm and the l^1 norm, and that it is positivity preserving with range the set of translation-invariant functions on 2^Λ.

Throughout this paper we choose the evolution of the system to be specified by the Glauber stochastic dynamics. This has the form

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

where

$$W(\omega, \omega') = \begin{cases} g(\omega)^{1/2} g(\omega')^{-1/2} & \text{if } \omega \sim \omega' \\ \sum_{\sigma \sim \omega'} g(\sigma)^{1/2} g(\omega')^{-1/2} & \text{if } \omega = \omega' \\ 0 & \text{otherwise} \end{cases} \tag{1.3}$$

so that

$$\sum_{\omega} W(\omega, \omega') = 0$$

for all $\omega' \in 2^\Lambda$. Three crucial features of this choice of dynamics are that g is stationary, that is

$$Wg = 0 \tag{1.4}$$

that W satisfies the detailed balance condition with respect to g, that is

$$W(\omega, \omega') g(\omega') = W(\omega', \omega) g(\omega)$$

for all $\omega, \omega' \in 2^\Lambda$, and that e^{Wt} is positivity preserving.

If the operator H on $L(X)$ is defined by

$$Hf(\theta\omega) = -g(\omega)^{-1} W(g \cdot f\theta)(\omega) \tag{1.5}$$

then

$$THf = -WTf \tag{1.6}$$

for all $f \in L(X)$, and we see from (1.4) that

$$H1 = 0$$

If $f, f' \in L(X)$ then

$$\begin{aligned} \int_X Hf(x) f'(x)\, dx &= \sum_{\omega} Hf(\theta\omega) f'(\theta\omega) g(\omega) \\ &= -\sum_{\omega} W(g \cdot f\theta)(\omega) f'(\theta\omega) \\ &= -\sum_{\omega, \omega'} W(\omega, \omega') f(\theta\omega') g(\omega') f'(\theta\omega) \\ &= -\sum_{\omega, \omega'} W(\omega', \omega) f(\theta\omega') g(\omega) f'(\theta\omega) \\ &= \int_X f(x) Hf'(x)\, dx \end{aligned}$$

Therefore H is self-adjoint. Moreover (1.6) implies that

$$Te^{-Ht}f = e^{Wt}Tf$$

for all $f \in L(X)$, so e^{-Ht} is a positivity preserving contraction semigroup on $L(X)$ for the L^1 norm, and hence also for the L^2 and L^∞ norms. Therefore the eigenvalues λ_n of H, repeated according to multiplicity, can be written in increasing order as

$$0 = \lambda_0 < \lambda_1 \leqslant \lambda_2 \leqslant \cdots$$

The eigenvalue $\lambda_0 = 0$ is nondegenerate because the semigroups e^{-Ht} and e^{Wt} are ergodic.

2. THE DEFINITION OF METASTABILITY

Having specified the model, we now investigate the existence of a metastable state. One of the first problems is that there are several different physical criteria for metastability, and that it was not very clear what the mathematical relationships between these criteria were. The contribution of Ref. 6 was to help clarify this point.

We take as fundamental to metastability the existence of two time scales for the evolution. The first time scale is the scale relevant to the relaxation of a small perturbation of the Gibbs state, while the second is the scale relevant to the relaxation of the metastable state (that is for the formation of a single supercritical droplet in the metastable state). It seems that in the present model the ratio of these two time scales may be of magnitude 10^{10} or even much bigger.

The simplest way in which these two time scales could be apparent would be if the eigenvalues λ_n of H satisfied

$$\lambda_1/\lambda_2 \equiv \epsilon \ll 1 \tag{2.1}$$

If there were several different metastable states, or some hidden symmetry, H would have a more complicated spectral structure. It was shown in Ref. 6 that subject to technicalities the spectral property (2.1) implies the existence of a partition of X into two regions M_1 and M_2, the smaller of which is called the metastable region M for the dynamics. The region M is nearly invariant under the dynamics in the sense that

$$\|e^{-Ht}\chi_M - \chi_M\|_1 \leqslant |M|\delta(1 + \lambda_2 t) \tag{2.2}$$

for all $t \geqslant 0$, where δ is a small constant, depending on ϵ. Thus the state $\chi_M/|M|$ is very nearly stationary on the time scale associated to λ_2 [which we call the normal time scale, choosing time units so that $\lambda_2^{\pm 1} = O(1)$]. The translation-invariant probability density q on 2^{Λ} defined by

$$q(\omega) = \begin{cases} g(\omega)|M|^{-1} & \text{if } \theta\omega \in M \\ 0 & \text{otherwise} \end{cases}$$

is then nearly stationary for the Glauber dynamics, and may be called the metastable state of the system.

According to the analysis of Ref. 6 the set M is defined as follows. If the eigenstate of H corresponding to the eigenvalue λ_1 is denoted by ϕ, then the self-adjointness of H implies that

$$0 = \langle \phi, 1 \rangle = \int_X \phi(x)\, dx$$

Therefore

$$M_1 = \{x : \phi(x) > 0\}$$
$$M_2 = \{x : \phi(x) \leqslant 0\}$$

both satisfy

$$0 < |M_i| < 1$$

and M is taken to be the set of smaller volume. The main point to notice here is that the set M is completely determined by the dynamics, and that no further physical input is necessary. Moreover the existence of a region M satisfying (2.2) is not only implied by the approximate degeneracy of the ground state in the sense of (2.1), but is actually *equivalent* to the approximate degeneracy of the ground state.

While the above analysis is very encouraging from the theoretical point of view, the difficulty of applying it to the Ising model is that it is very hard to determine the eigenvalues λ_1 and λ_2 or the eigenvector ϕ explicitly. It has therefore been the practice in the physical literature[1,2,8,10] to write down conditions involving "critical sized droplets" which specify a set N of configurations with the status of an approximate metastable region. The calculations of Refs. 2 and 11 provide strong evidence that the set N is very close to M in some sense.

Because the computations involved in the above procedure are very complicated, Davies and Martin[7] introduced another proposal for defining the metastable state, which amounts to replacing χ_M by a function K on X which should be approximately equal to one inside M and approximately equal to zero outside M. This new procedure leads to less accurate approximations than that mentioned in the last paragraph, but has the compensating virtue of involving rather simpler computations. The function K satisfies

$$0 < K(x) \leqslant 1$$

for all $x \in X$, and the corresponding metastable state on 2^{Λ} is defined by

$$q(\omega) = aK(\theta\omega)\, g(\omega) \tag{2.3}$$

where

$$a^{-1} = \sum_{\omega} K(\theta\omega) g(\omega) = \int_X K(x)\, dx$$

The actual definition of K is given in terms of a suitable perturbation $\mathcal{V}_x$ of the Hamiltonian $\mathcal{H}_0$, namely,

$$K(\theta\omega) = \exp\left[-\beta\alpha\mathcal{V}_x(\omega)\right] \tag{2.4}$$

The trick is to choose $\alpha > 0$ and $\mathcal{V}_x$ so as to make $K(x)$ as near to one inside M and as near to zero outside M as possible. The restriction to two-body forces in $\mathcal{V}_x$ is made in Ref. 7 to ensure a computationally simple scheme, and by allowing higher-order interactions one could obtain approximations of considerably greater accuracy.

The procedure of replacing the characteristic function χ_M of the metastable region M by a function K, satisfying $0 \leqslant K(x) \leqslant 1$ for all $x \in X$, has been discussed at a mathematical level in Ref. 6, Section 3. It was shown there that if K satisfies

$$\| e^{-Ht} K - K \|_1 \leqslant \delta \| K \|_1 t$$

for all $t \geqslant 0$ and some $\delta = o(1)$, as well as some further technically nontrivial conditions, and if N is defined by

$$N = \{ x \in X : K(x) \geqslant \tfrac{1}{2} \}$$

then

$$\| e^{-Ht} \chi_N - \chi_N \|_1 \leqslant \delta' |N| (1 + t)$$

where $\delta' = o(1)$. Thus N is an approximation to the metastable region. We shall see in Section 5 that these conditions on K are satisfied for the choice (2.4) of K with $\mathcal{V}_x$ as specified in the next section.

3. THE CHOICE OF $\mathcal{V}_x$

It was shown in Ref. 7 that if one minimizes the free energy of the Ising model subject to a quadratic constraint on the magnitude of the spin wave fluctuations, one is led to the choice

$$\mathcal{V}_x = \sum_{i,j \in \Lambda} w_p(i-j)(\sigma_i - x)(\sigma_j - x) = -2x\mathcal{V} + x^2|\Lambda| \tag{3.1}$$

where

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

and the value of x is determined by a procedure described below. The periodic function w_p is characteristic of the constraint chosen, and is determined by a summable function $w : \mathbb{Z}^d \to \mathbb{R}$ according to the equation

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

We shall generally not distinguish notationally between w and w_p. We shall not write down the conditions on w obtained in Ref. 7, but throughout this paper content ourselves with the particular choice

$$w(i) = ce^{-i^2/2\gamma^2}$$

where

$$c^{-1} = \sum_{j \in \mathbb{Z}^d} e^{-j^2/2\gamma^2}$$

Although we shall later choose γ to depend upon μ according to

$$\gamma = \gamma_1 \mu^{-1/d}$$

we content ourselves at present with the restriction

$$1 \ll \gamma^d \ll |\Lambda| \tag{3.2}$$

which ensures that $\mathcal{V}$ has range which is long compared with the lattice spacing but short compared to the size of the box. Under this restriction we see that

$$\|w_p\|_\infty \sim \|w\|_\infty = c \sim (2\pi)^{-d/2} \gamma^{-d}$$

Moreover for large γ

$$\sum_{i \in \mathbb{Z}^d} |i| w(i) \sim c'\gamma$$

If we rewrite

$$(\mathcal{H}_0 - \mu \mathfrak{M}) + \alpha \mathcal{V}_x = (\mathcal{H}_0 + \alpha \mathcal{V}) - (\mu + 2\alpha x)\mathfrak{M} + \alpha x^2 |\Lambda|$$

then we see from (2.3) and (2.4) that q is the Gibbs state

$$q = \exp[-\beta(\mathcal{H} - \nu \mathfrak{M})] / \sum_{\omega'} \exp\{-\beta[\mathcal{H}(\omega') - \nu \mathfrak{M}(\omega')]\} \tag{3.3}$$

of the modified Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \alpha \mathcal{V}$$

in the effective external field

$$\nu = \mu + 2\alpha x$$

The free energy functional Φ^Λ of this Hamiltonian is defined by

$$\Phi^\Lambda(\nu) = -(\beta|\Lambda|)^{-1}\log \operatorname{tr}\exp[-\beta(\mathcal{H} - \nu\mathfrak{M})]$$

while if we parametrize by the magnetization x instead of the external field ν we obtain

$$\Psi^\Lambda(x) = |\Lambda|^{-1}\min\{\operatorname{tr}[\mathcal{H}\rho] - \beta^{-1}S(\rho) : \operatorname{tr}[\sigma\rho] = x\} = \Phi^\Lambda(\nu) + \nu x$$

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

$$\frac{\partial \Phi^\Lambda(\nu)}{\partial \nu} = -x$$

The thermodynamic limits of Φ^Λ and Ψ^Λ as $N \to \infty$ (so that $\Lambda \to \infty$ in the sense of van Hove) are denoted by Φ and Ψ.

The analysis in Ref. 7 depends upon several hypotheses concerning the thermodynamic behavior of the Hamiltonians $\mathcal{H}$ and $\mathcal{H}_0$. These hypotheses are supported by all known results concerning two-body interactions on lattices, but have not yet been rigorously proved to hold.

(H1) For small enough $\alpha > 0$ the spontaneous magnetization $m = m(\alpha, \gamma)$ of $\mathcal{H}$ is less than the spontaneous magnetization m_0 of $\mathcal{H}_0$. Moreover for fixed γ, $m \to m_0$ as $\alpha \to 0+$.

(H2) For small enough $\alpha > 0$ the free energy functional $\Psi(x)$ of $\mathcal{H}$ satisfies

$$\Psi(x) = f \qquad \text{if} \quad -m \leqslant x \leqslant m$$

where f depends on α, γ. Moreover $\Psi(x)$ is analytic for $|x| > m$ and is differentiable at $x = \pm m$ with $\Psi'(\pm m) = 0$.

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

(H4) Let $\phi_{0,\nu}^\Lambda$ denote the two-point function for the Hamiltonian $\mathcal{H}_0$ in the volume Λ for the field ν, so that

$$\phi_{0,\nu}^\Lambda(i-j) = \langle(\sigma_i - \langle\sigma_i\rangle)(\sigma_j - \langle\sigma_j\rangle)\rangle_{\Lambda,\mathcal{H}_0,\beta,\nu}$$

Then the associated Gibbs states are uniformly L^1 clustering as $\Lambda \to \infty$ for each $\nu \neq 0$, in the sense that there exists a constant $c_0 < \infty$ such that

$$\|\phi_{0,\nu}^\Lambda\|_1 \leqslant c_0 < \infty$$

for each $\nu \neq 0$ and all large enough Λ.

(H5) The same as (H4) except that $\mathcal{H}_0$ is replaced by $\mathcal{H}$, $\phi_{0,\nu}^\Lambda$ by ϕ_ν^Λ, and c_0 by c.

(H6) There exist constants k and n such that if $\nu \neq 0$ then

$$\|\phi_\nu^\Lambda\|_1 \leqslant k^2 m(\alpha, \gamma)^{-n} \tag{3.4}$$

for all large enough Λ. Note that if $\nu \neq 0$ is very small then (3.4) can only hold for correspondingly large Λ, because of the phase transition which occurs at $\nu = 0$.

We shall not repeat the thermodynamic arguments which led us in Ref. 7 to the choice (3.1) of $\mathcal{V}_x$ and the choice (3.3) of q. In the calculations of Ref. 7, and also here, the constraint

$$\mathrm{tr}[\sigma_i q] = x$$

on x is fundamental. The magnetization x and the effective field ν are thus always determined from μ, α, γ by the equations

$$\nu = \mu + 2\alpha x, \qquad \frac{\partial \Phi}{\partial \nu} = -x \tag{3.5}$$

If α is small then there is always a solution of these equations with $x \doteqdot m_0(\mu)$ and this yields (an approximation to) the Gibbs state g. However if

$$2\alpha m(\alpha, \gamma) > \mu \tag{3.6}$$

then it was shown in Ref. 7 that there is a second solution of (3.5) with $\nu < 0$ and $x < 0$. The corresponding state was shown to have a fairly long lifetime and was interpreted as a metastable state of the system.

4. THE METASTABLE REGION FOR $\mathcal{V}_x$

Although the physical motivation for the above choice of $\mathcal{V}_x$ was, to our mind, adequately presented in Ref. 7, its relationship to better established approaches to metastability is admittedly not clear. In this section we attempt to bridge this gap by evaluating $K(x)$ for some typical configurations of the spins, in order to gain a qualitative impression of its effect.

Throughout this section we take $\beta = 1$; this does not decrease the generality since the factor β may always be absorbed into other parameters, such as J and μ, and it makes the formulas below simpler to appreciate. Since

$$K(\theta\omega) = \exp[-\alpha \mathcal{V}_x(\omega)]$$

where $\mathcal{V}_x(\omega) \geqslant 0$ for all configurations ω, we see that $K(\theta\omega)$ is approximately equal to 1 or 0 when $\alpha\mathcal{V}_x(\omega)$ is approximately equal to 0 or $+\infty$, respectively.

It is necessary for our purpose to let α and γ depend on μ in such a way that (3.2), (3.6), (4.4), (4.5), (4.6) all hold. The condition (3.6) was discussed in Ref. 7 for the model form

$$m(\alpha, \gamma) = m_0 - m_1 \alpha\gamma$$

It was also shown in Ref. 9, p. 114, that $m(\alpha,\gamma) > 0$ provided $\alpha\gamma$ is small enough. It may be seen that possible choices of α and γ are given by (4.1) below.

(H7) There exist constants α_1, γ_1 such that if

$$\alpha = \alpha_1 \mu, \qquad \gamma = \gamma_1 \mu^{-1/d} \tag{4.1}$$

then

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

for all sufficiently small $\mu > 0$.

If $\omega \in 2^\Lambda$ is any configuration, its magnetization density $\bar{x}$ is defined by

$$\bar{x} = |\Lambda|^{-1} \sum_{i\in\Lambda} \sigma_i$$

while its two-point function $b_i : \Lambda \to \mathbb{R}$ is defined by

$$b_i = \frac{1}{|\Lambda|} \sum_{j\in\Lambda} (\sigma_{i+j} - \bar{x})(\sigma_j - \bar{x})$$

The configuration is said to have normal fluctuations if

$$b \equiv \sum_{i\in\Lambda} |b_i| = O(1)$$

Lemma 1. For every configuration $\omega \in 2^\Lambda$ we have

$$\alpha_1 \mu (x - \bar{x})^2 |\Lambda| \leqslant \alpha \mathcal{V}_x(\omega) \leqslant \alpha_1 \mu (x - \bar{x})^2 |\Lambda| + (2\pi)^{-d/2} \gamma_1^{-d} \alpha_1 \mu^2 b |\Lambda|$$

Thus $\alpha \mathcal{V}_x(\omega) = o(1)$ implies

$$\mu (x - \bar{x})^2 |\Lambda| = o(1) \tag{4.2}$$

and is implied by this together with

$$\mu^2 |b| \Lambda| = o(1) \tag{4.3}$$

Proof. By definition

$$\begin{aligned}
\mathcal{V}_x(\omega) &= \sum_{i,j} w_{i-j} (\sigma_i - x)(\sigma_j - x) \\
&= \sum_{i,j} w_i \sigma_{i+j} \sigma_j - 2x\bar{x}|\Lambda| + x^2|\Lambda| \\
&= \sum_i w_i \big(b_i|\Lambda| + \bar{x}^2|\Lambda| \big) - 2x\bar{x}|\Lambda| + x^2|\Lambda| \\
&= \sum_i w_i b_i |\Lambda| + (x - \bar{x})^2 |\Lambda|
\end{aligned}$$

Moreover

$$\sum_i w_i b_i |\Lambda| = \sum w_{i-j}(\sigma_i - \bar{x})(\sigma_j - \bar{x}) \geqslant 0$$

because w is of positive type. Therefore

$$\alpha(x-\bar{x})^2|\Lambda| \leqslant \alpha \mathcal{V}_x(\omega) \leqslant \alpha(x-\bar{x})^2|\Lambda| + \alpha b\|w\|_\infty|\Lambda|$$

from which the result follows by applying (4.1).

The above lemma implies that if

$$\lambda^{-1} \ll |\Lambda| \ll \lambda^{-2} \tag{4.4}$$

then the weight $K(\theta\omega)$ of configuration ω is very small unless $x \doteqdot \bar{x}$, and if this holds then the weight is nearly one if the configuration has normal fluctuations.

The presence of the factor $|\Lambda|$ in (4.2) and (4.3) is disturbing at first, because it suggests that the volume of the system cannot be taken too large. However, the same problem occurs in the orthodox approach to metastability, not at the stage of defining the metastable region but at the stage of evaluating its lifetime. The physical reason is that there is a constant rate of nucleation per unit volume, so that the global lifetime is inversely proportional to the volume. See Refs. 10 and 11 for a treatment in which the thermodynamic limit may nevertheless be taken for these problems by limiting the class of observed quantities.

Our next step is to estimate $\mathcal{V}_x(\omega)$ for a configuration ω consisting of a droplet of charges $+1$ and radius r embedded in a background of magnetization density $x < 0$ with normal fluctuations. Because this computation is rather messy we refer to (3.2) to justify the simplification of replacing σ_i by a continuous distribution $\sigma(u)$ on $\mathbb{R}^d$ given by

$$\sigma(u) = x + (1-x)e^{-u^2/r^2}$$

so that r determines the scale of the charge reversal region. In this approximation $\mathcal{V}_x(\omega)$ equals

$$\begin{aligned}
&\int_{\mathbb{R}^d\times\mathbb{R}^d} (2\pi)^{-d/2}\gamma^{-d}\exp\left[-(u-v)^2/2\gamma^2\right]\left[\sigma(u)-x\right]\left[\sigma(v)-x\right]d^du\,d^dv \\
&\quad = (1-x)^2\int_{\mathbb{R}^d\times\mathbb{R}^d}(2\pi)^{-d/2}\gamma^{-d} \\
&\qquad \times \exp\left[-(u-v)^2/2\gamma^2 - u^2/r^2 - v^2/r^2\right]d^du\,d^dv \\
&\quad = 2^{-d/2}\pi^{d/2}r^{2d}\left(\gamma^2+r^2\right)^{-d/2}
\end{aligned}$$

If α and γ are defined by (4.1) and we put $r=\gamma$ we obtain

$$\alpha\mathcal{V}_x(\omega) = 2^{-d}\pi^{d/2}\gamma^d\alpha = 2^{-d}\pi^{d/2}\alpha_1\gamma_1 \equiv b \tag{4.5}$$

which is neither very small nor very large. If $r < \gamma$ then

$$\alpha \mathcal{V}_x(\omega) \leqslant 2^{-d}\pi^{d/2} r^d \alpha = b\left(\frac{r}{\gamma}\right)^d$$

while if $r > \gamma$ then

$$\alpha \mathcal{V}_x(\omega) \geqslant 2^{-d}\pi^{d/2} r^d \alpha = b\left(\frac{r}{\gamma}\right)^d$$

We thus see that the weight $\exp[-\alpha \mathcal{V}_x(\omega)]$ of the configuration is nearly 1 if $r \ll \gamma$ and nearly 0 if $r \gg \gamma$, so that the critical droplet radius in this model is

$$r_c \sim \gamma \tag{4.6}$$

This is quantitatively different from the correct form $r_c \sim \mu^{-1}$, but has the correct qualitative behavior as $\mu \to 0$. Note that (3.2) ensures that the volume of the critical droplet is much less than $|\Lambda|$.

5. STABILITY AND LIFETIME

Continuing with the notation of Sections 1 and 2 we now consider the problems of the stability and lifetime of a metastable state with respect to the symmetric Markov semigroup e^{-Ht} on $L(X)$. We suppose that this state is determined by the density $\rho = aK$ on X where

$$a^{-1} = \int_X K(y)\, dy$$

and

$$0 < K(x) \leqslant 1$$

for all $x \in X$. Our subsequent calculations will only be valuable if $K(x) \doteqdot 1$ for x inside the metastable region M and $K(x) \doteqdot 0$ for x outside M, with the possible exception of a small transition region. Our following remarks paraphrase theorems in Ref. 6.

In order to justify calling ρ a metastable state one has first to show that it has a very long lifetime, or alternatively that $e^{-Ht}\rho$ varies very slowly. One also has to show that ρ is stable, in the sense that if η is a small perturbation of ρ then η converges to ρ on a short time scale before eventually moving with ρ to the final equilibrium state 1. We consider the probability density η to be a small perturbation of ρ if

$$0 \leqslant \eta \leqslant c\rho$$

for some $c = O(1)$. One necessarily has $c \geqslant 1$, and the assumption that c is not too large prevents η from being concentrated almost entirely near the boundary of the metastable region M.

In order to examine the above questions it is convenient to introduce another evolution on $L(X)$, for which ρ is an exact stationary state. If we define $\tilde{H}$ on $L(X)$ by

$$\tilde{H}(f) = \rho^{1/2}H(\rho^{-1/2}f) - \rho^{-1/2}H(\rho^{1/2})f \tag{5.1}$$

then it follows by Ref. 6, Theorem 13 that $e^{-\tilde{H}t}$ is a positivity-preserving semigroup on $L(X)$ such that

$$\tilde{H}\rho = 0$$

and

$$\int_X e^{-\tilde{H}t}f(x)\,dx = \int_X f(x)\,dx$$

for all $f \in L(X)$ and $t \geqslant 0$.

The motivation for this definition (5.1) of $\tilde{H}$ is provided by the following lemma.

Lemma 2. If $\tilde{W}$ is the generator of the Glauber stochastic dynamics on 2^Λ corresponding to the metastable state

$$q(\omega) = aK(\theta\omega)\,g(\omega) = \rho(\theta\omega)\,g(\omega) \tag{5.2}$$

then

$$Te^{-\tilde{H}t}f = e^{\tilde{W}t}Tf \tag{5.3}$$

for all $t \geqslant 0$ and $f \in L(X)$.

Proof. The formula (5.3) is equivalent to

$$T\tilde{H}f = \tilde{W}Tf$$

which may be written explicitly as

$$\tilde{H}f(\theta\omega) = -g(\omega)^{-1}\tilde{W}(g \cdot f\theta)(\omega)$$

The definition of $\tilde{W}$ is

$$\tilde{W}(\omega,\omega') = \begin{cases} q(\omega)^{1/2}q(\omega')^{-1/2} & \text{if } \omega \sim \omega' \\ -\sum\limits_{\sigma\sim\omega'} q(\sigma)^{1/2}q(\omega')^{-1/2} & \text{if } \omega = \omega' \\ 0 & \text{otherwise} \end{cases} \tag{5.4}$$

It is clear from (1.3) and (5.4) that

$$\tilde{W}(\omega,\omega') = K(\theta\omega)^{1/2}W(\omega,\omega')K(\theta\omega')^{-1/2}$$

if $\omega \neq \omega'$. On the other hand

$$
\begin{aligned}
(H\rho^{1/2})(\theta\omega) &= -g(\omega)^{-1} W\big(a^{1/2}(K\theta)^{1/2} g\big)(\omega) \\
&= -\sum_{\omega\sim\omega'} g(\omega)^{-1} g(\omega)^{1/2} g(\omega')^{-1/2} a^{1/2} K(\theta\omega')^{1/2} g(\omega') \\
&\quad + \sum_{\sigma\sim\omega} g(\omega)^{-1} g(\sigma)^{1/2} g(\omega)^{-1/2} a^{1/2} K(\theta\omega)^{1/2} g(\omega) \\
&= -\sum_{\omega\sim\omega'} g(\omega)^{-1/2} q(\omega')^{1/2} \\
&\quad + \sum_{\sigma\sim\omega} g(\sigma)^{1/2} g(\omega)^{-1/2} a^{1/2} K(\theta\omega)^{1/2}
\end{aligned}
$$

Therefore

$$
\begin{aligned}
(\rho^{-1/2} H \rho^{1/2})(\theta\omega) &= -\sum_{\omega\sim\omega'} q(\omega)^{-1/2} q(\omega')^{1/2} + \sum_{\sigma\sim\omega} g(\sigma)^{1/2} g(\omega)^{-1/2} \\
&= \tilde{W}(\omega,\omega) - W(\omega,\omega)
\end{aligned}
$$

Therefore

$$
\tilde{W}(\omega,\omega') - K(\theta\omega)^{1/2} W(\omega,\omega') K(\theta\omega')^{-1/2} = \delta_{\omega\omega'}(\rho^{-1/2} H \rho^{1/2})(\theta\omega)
$$

for all $\omega, \omega' \in 2^{\Lambda}$, and

$$
\begin{aligned}
(\tilde{H} f)(\theta\omega) &= \left[\rho^{1/2} H(\rho^{-1/2} f)\right](\theta\omega) - (\rho^{-1/2} H \rho^{1/2})(\theta\omega) f(\theta\omega) \\
&= -\rho(\theta\omega)^{1/2} g(\omega)^{-1} W(g \cdot \rho^{-1/2}\theta \cdot f\theta)(\theta\omega) \\
&\quad - (\rho^{-1/2} H \rho^{1/2})(\theta\omega) f(\theta\omega) \\
&= -g(\omega)^{-1} \tilde{W}(g \cdot f\theta)(\theta\omega)
\end{aligned}
$$

as required.

Our central claim is that positive information concerning the stability and lifetime of ρ is provided if whenever

$$
0 \leqslant \eta \leqslant c\rho
$$

we have

$$
\| e^{-Ht}\eta - e^{-\tilde{H}t}\eta \|_1 \leqslant \epsilon c t \tag{5.5}
$$

for all $t \geqslant 0$, where $\epsilon = o(1)$. If this is valid then *although* the ergodicity of e^{-Ht} implies that

$$
\lim_{t\to\infty} \| e^{-Ht}\eta - 1 \|_1 = 0
$$

it *appears* that

$$
\lim_{t\to\infty} \| e^{-Ht}\eta - \rho \|_1 = 0 \tag{5.6}
$$

if one restricts to times $t = o(\epsilon^{-1})$. We leave open the problem of determining for which η one can be sure that the convergence of $e^{-\tilde{H}t}\eta$ to ρ is fairly rapid. As a special case of (5.5) we do, however, see that

$$\|e^{-Ht}\rho - \rho\|_1 \leqslant \epsilon t$$

for all $t \geqslant 0$, so the state ρ certainly has a long lifetime.

It was shown in Ref. 6, Theorem 15 that (5.5) holds provided

$$\|(H - \tilde{H})\rho f\|_1 \leqslant \epsilon \|f\|_\infty$$

for all $f \in L^\infty(X)$. Since the map T defined in (1.2) is isometric this is equivalent to

$$\|(W - \tilde{W})T(\rho f)\|_1 \leqslant \epsilon \|f\|_\infty$$

and is implied by

$$\|(W - \tilde{W})fq\|_1 \leqslant \epsilon \|f\|_\infty$$

for all $f \in l^\infty(2^\Lambda)$.

Theorem 3. There exists a constant c such that

$$\|(W - \tilde{W})fq\|_1 \leqslant c\mu^{3/2}|\Lambda| \|f\|_\infty$$

for all $f \in l^\infty(2^\Lambda)$.

We defer the proof of this theorem to Section 6, since it is rather technical and depends upon the detailed notation of Ref. 7. We see that we have an upper bound on the decay rate

$$\epsilon = c\mu^{3/2}|\Lambda| \tag{5.7}$$

which does not remain small in the thermodynamic limit $|\Lambda| \to \infty$, for reasons already stated. However, for fixed $|\Lambda|$ it is the case that ϵ is very small if μ is very small.

It is rather disappointing that the upper bound (5.7) on the decay rate is much larger than that obtained in Ref. 2, but we wish to emphasize that this *may* be just a result of the crudity of our estimation procedure. It may alternatively be an intrinsic limitation due to the use of a two-body potential $\mathcal{V}$. We also emphasize that no proof of stability of the metastable state such as (5.6) has been obtained using the standard definition of metastability.

We stated at the end of Section 2 that it is possible to obtain an approximate metastable region N from the probability density q under certain extra technical conditions. These extra conditions are stated in Ref. 6, Theorem 7. Making the identification

$$\sigma(\theta\omega) = \beta\alpha\mathcal{V}_x(\omega)$$

so that the symbol ρ stands for the same entity as in this paper, the condition (ii) of Ref. 6, Theorem 7 is a trivial consequence of Ref. 7, Lemma 5, while condition (iii) of Ref. 6, Theorem 7 amounts to the assumption that the expected value

$$\sum_{\omega} \beta\alpha \mathcal{V}_x(\omega) q(\omega)$$

of σ in the metastable state q is very small. But it was shown in the proof of Ref. 7, Theorem 8 that

$$\sum_{\omega} \beta\alpha \mathcal{V}_x(\omega) q(\omega) \leqslant \beta\alpha|\Lambda| \left\{ \|w\|_\infty \|\phi^\Lambda\|_1 + (x^\Lambda - x)^2 \right\} \leqslant c\mu^2|\Lambda|$$

We thus see that if

$$\mu^2|\Lambda| = O(1) \tag{5.8}$$

then by Ref. 6, Theorem 7 the set

$$N = \{ x \in X : K(x) \geqslant 1/2 \}$$

is an approximate metastable region. Alternatively the set

$$N' = \{ \omega \in 2^\Lambda : \beta\alpha \mathcal{V}_x(\omega) \leqslant \log 2 \} \tag{5.9}$$

is an approximate metastable region in 2^Λ.

We finally summarize our hypotheses on μ, α, γ, and $|\Lambda|$. We assumed in (4.1) that

$$\alpha = \alpha_1 \mu, \qquad \gamma = \gamma_1 \mu^{-1/d}$$

while in (3.2) and (4.4) we needed the estimates

$$\mu^{-1} \ll |\Lambda| \ll \mu^{-2}$$

in order to obtain physically sensible results. We then concluded in (4.6) that the critical droplet radius is

$$r_c \sim \gamma$$

and that there is a metastable region N' in 2^Λ given by (5.9). The most unsatisfactory result was that we were only able to obtain the upper bound

$$\epsilon = c\mu^{3/2}|\Lambda|$$

to the decay rate (5.7).

6. PROOF OF THEOREM 3

Our proof of Theorem 3 must be read in conjunction with Lemmas 6 and 7 of Ref. 7, which were proved for a similar purpose but with a less powerful result in mind. We summarize the notation we are using, which is almost the same in both papers. The Gibbs state g on 2^Λ is defined by (1.1) and the function K on 2^Λ by

$$K(\omega) = \exp\left[-\beta\alpha\mathcal{V}_x(\omega)\right]$$

while the normalization constant a is

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

and the metastable state q is given by

$$q(\omega) = aK(\omega)\,g(\omega) = \rho(\omega)\,g(\omega)$$

The two stochastic kernels W and $\tilde{W}$ are defined by (1.3) and (5.4).

If $f \in l^\infty(2^\Lambda)$ and $\omega \in 2^\Lambda$ then

$$\begin{aligned}
&\{(W-\tilde{W})fq\}(\omega)\\
&\quad= \sum_{\omega'\sim\omega}\{W(\omega,\omega')f(\omega')q(\omega') - \tilde{W}(\omega,\omega')f(\omega')q(\omega')\}\\
&\qquad + W(\omega,\omega)f(\omega)q(\omega) - \tilde{W}(\omega,\omega)f(\omega)q(\omega)\\
&\quad= \sum_{\omega'\sim\omega}\{W(\omega,\omega')f(\omega')q(\omega') - \tilde{W}(\omega,\omega')f(\omega')q(\omega')\\
&\qquad\qquad - W(\omega',\omega)f(\omega)q(\omega) + \tilde{W}(\omega',\omega)f(\omega)q(\omega)\}\\
&\quad= \sum_{\omega'\sim\omega}\{g(\omega)^{1/2}g(\omega')^{1/2}f(\omega')aK(\omega')\\
&\qquad\qquad - g(\omega)^{1/2}g(\omega')^{1/2}f(\omega')aK(\omega)^{1/2}K(\omega')^{1/2}\\
&\qquad\qquad - g(\omega)^{1/2}g(\omega')^{1/2}f(\omega)aK(\omega)\\
&\qquad\qquad + g(\omega)^{1/2}g(\omega')^{1/2}f(\omega)aK(\omega')^{1/2}K(\omega)^{1/2}\}
\end{aligned}$$

Therefore

$$\begin{aligned}
&\|(W-\tilde{W})fq\|_1/\|f\|_\infty\\
&\qquad \leqslant 2a\sum_{\omega\sim\omega'} g(\omega)^{1/2}g(\omega')^{1/2}K(\omega)^{1/2}|K(\omega)^{1/2} - K(\omega')^{1/2}|
\end{aligned}$$

Now

$$|K(\omega)^{1/2} - K(\omega')^{1/2}| \leqslant \tfrac{1}{2}\,\beta\alpha\max\{K(\omega)^{1/2}, K(\omega')^{1/2}\}|\mathcal{V}_x(\omega) - \mathcal{V}_x(\omega')|$$

and by the proof of Lemma 6 of Ref. 7

$$g(\omega')^{1/2} \leqslant g(\omega)^{1/2}\exp\left[\beta(\mu + 2\|h\|_1)\right]$$

$$\max\left\{K(\omega)^{1/2}, K(\omega')^{1/2}\right\} \leqslant K(\omega)^{1/2}\exp(4\beta\alpha)$$

Therefore

$$\|(W - \tilde{W})fq\|_1/\|f\|_\infty \leqslant a\beta\alpha \sum_{\omega\sim\omega'} g(\omega)K(\omega)|\mathcal{V}_x(\omega) - \mathcal{V}_x(\omega')|$$

$$= \beta\alpha\sum_{\omega} q(\omega)Y(\omega)$$

where

$$Y(\omega) = \sum_{\omega'\sim\omega} |\mathcal{V}_x(\omega) - \mathcal{V}_x(\omega')|$$

as in Ref. 7, Lemma 6. By Ref. 7, Lemma 7 we deduce that

$$\sum_{\omega} q(\omega)Y(\omega) \leqslant 4|\Lambda|w(0) + 4|\Lambda|^{1/2}\left\{\sum_{\omega}\mathcal{V}_x(\omega)q(\omega)\right\}^{1/2}$$

and then by the proof of Ref. 7, Theorem 8

$$\sum_{\omega}\mathcal{V}_x(\omega)q(\omega) \leqslant |\Lambda|\left\{\|w\|_\infty\|\phi^\Lambda\|_1 + (x^\Lambda - x)^2\right\}$$

The statement of our theorem follows by combining the above estimates with the estimates

$$\alpha = O(\mu), \qquad \|w\|_\infty = O(\mu)$$

resulting from (4.1).

ACKNOWLEDGMENTS

It is my great pleasure to thank Ph. A. Martin and G. Sewell for many valuable conversations and letters concerning metastability and O. Penrose for valuable criticisms of the manuscript.

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