

# Metastability: from mean field models to spdes

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**Abstract** Kramer's equation of a diffusion in a double well potential has been the paradigm for a metastable system since 1940. The theme of this note is to partially explain, why and in what sense this is a good model for metastable systems. In the process, I review recent progress in a variety of models, ranging from mean field spin systems to stochastic partial differential equations.

## 1 Introduction

Metastability is in essence the dynamical signature of a first order phase transition in statistical mechanics. In equilibrium statistical mechanics, a first order phase transition is said to occur if a system is very sensitive to the change of a parameter (resp. boundary conditions), in the sense that an extensive variable (e.g. density or magnetization) shows a discontinuity as functions of some intensive variable (e.g. pressure or magnetic field), in the thermodynamics limit. Dynamically, for a finite system, this fact manifests itself in that as the parameter is varied across the phase transition line, the system will remain a considerable (and mostly random) amount of time in the "wrong phase" before suddenly changing into the true equilibrium phase (in other words, the sensitive variable will change its value as a function of time with a random delay).

Metastability is a very widespread phenomenon that occurs in a large variety of systems, both natural and artificial. In many instances, it has important effects that are crucial for the proper functioning of the system and there has been great interest in understanding metastability in quantitative terms over at least the last century.

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Most metastable systems of practical relevance are many-body systems whose dynamics is very hard to analyze, both analytically and numerically. This is particularly true with respect to metastability, due to the very long time scales that are involved.

One of the first *mathematical models* for metastability was proposed in 1940 by Hendrik Anthony Kramers [25]. It consists of the simple, one-dimensional diffusion equation

$$dX_t = b(X_t)dt + \sqrt{2\varepsilon}dB_t, \quad (1)$$

where  $b(x) = -V'(x)$ , with  $V(x)$  a *double well potential*, i.e. a function with two local minima that tends to infinity at  $\pm\infty$ , and  $B_t$  is Brownian motion. In fact, this equation emerged as a special case of the more general equations he considered, namely

$$\mu^{-1}X_t'' = -X_t' + b(X_t) + \sqrt{2\varepsilon}B_t', \quad (2)$$

in the limit  $\mu \uparrow \infty$ . Thus Kramers' equation (1) can be seen as the equation of motion of a particle moving under the influence of a gradient force and a random force with friction in the limit where the friction becomes infinitely strong.

Kramers' equation (1) has become the paradigm of metastability. Kramers had been able to solve all interesting questions in the context of this model. In particular, he derived the so called *Kramers-formula* for the average transition time,  $\mathbb{E}_a \tau_b$ , from a minimum at  $a$ , via the maximum,  $z^*$ , to the minimum,  $b$ , as

$$\mathbb{E}_a \tau_b = \frac{2\pi}{\sqrt{V''(a)V''(z^*)}} \exp(\varepsilon^{-1}(V(z^*) - V(a))) (1 + o(1)). \quad (3)$$

The multi-dimensional generalization of this formula is attributed to Eyring and called *Eyring-Kramers formula* (see also [39]). Note that Eyring's so-called *reaction rate theory* [22] is based on quantum mechanical considerations and quite different from the classical theory of Kramers, although it appears to have the idea of interpreting  $V$  as a restricted (quantum mechanical) free energy in it. For a historical discussion, see the recent paper by Pollak and Talkner [35].

The question I want to discuss in this paper is how one may understand that indeed this simple equation can reflect quite properly the metastable behavior of the complex dynamics of many-body systems.

Before entering into any further discussion, we need to talk about the dynamics of many-body systems we want to discuss.

## 1.1 Stochastic Ising models

To analyse in any sense of rigour the microscopic dynamics of many-body systems as given by Newton's laws or even by the many-body Schrödinger equation is analytically beyond today's technology. A reasonable compromise, to which I will stick here, are stochastic Ising models. Here the setting is the following: we consider a

state space  $\mathcal{S}_\Lambda \equiv \{-1, +1\}^\Lambda$ , with  $\Lambda \subset \mathbb{Z}^d$  a finite subset of a lattice. A configuration  $\sigma \in \mathcal{S}_\Lambda$  describes the values of the magnetic moments of the atoms placed at the sites of  $\Lambda$ , in the magnetic interpretation. Alternatively, one may think of a *lattice gas* in which case the variables  $(1 + \sigma_i)/2$  represent the number of particles on the site  $i$ .

The interaction of the model is described by a *Hamiltonian*,  $H_\Lambda : \mathcal{S}_\Lambda \rightarrow \mathbb{R}$ , which is a real valued function on configuration space representing the *energy* of a configuration.

By *Glauber dynamics* I will mean a Markov chain (in continuous or discrete time) with transitions rates  $p(\sigma, \sigma')$  that are reversible with respect to the *Gibbs measure*,  $\mu_{\beta, \Lambda}$ , given by<sup>1</sup>

$$\mu_{\beta, \Lambda}(\sigma) \equiv \frac{1}{Z_{\beta, \Lambda}} \exp(-\beta H_\Lambda(\sigma)). \quad (4)$$

I will assume the dynamics to be local, in the sense that  $p(\sigma, \sigma')$  are non-zero only if  $\sigma$  and  $\sigma'$  differ in at most one site. One may of course think of many similar, but different, situations.

In this context, the extensive variable one would like to consider is the *magnetisation*,

$$m_\Lambda(\sigma) \equiv \frac{1}{|\Lambda|} \sum_{i \in \Lambda} \sigma_i. \quad (5)$$

Under reasonable assumptions on the Hamiltonian, the random variable  $m_\Lambda$  satisfies a *large deviation principle* under the Gibbs measure, i.e.

$$\mu_{\beta, \Lambda}(m_\Lambda(\sigma) = m) \sim \exp(-\Lambda \beta f_\beta(m)), \quad (6)$$

where the rate function  $f_\beta$  is called the *free energy*. A first order phase transition occurs when  $f_\beta$  is not strictly convex. Can we interpret Kramers' equation as an approximation of the behavior of  $m_\Lambda(\sigma(t))$ , when  $\sigma(t)$  is a Glauber dynamics for our model? This is loosely speaking the issue around which this note will turn.

## 2 The Curie-Weiss model

There is a simple model where all works well, the Curie-Weiss model of a ferromagnet. Here the Hamiltonian is very simple, namely

$$H_\Lambda(\sigma) \equiv -\frac{|\Lambda|}{2} (m_\Lambda(\sigma))^2 = -\frac{1}{2|\Lambda|} \sum_{i, j \in \Lambda} \sigma_i \sigma_j. \quad (7)$$

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<sup>1</sup> Note that I will not seriously enter the discussion of infinite volume dynamics and so I also do not enter the formalism of infinite volume Gibbs measures.

Since the form of  $\Lambda$  does not enter here, let us fix  $\Lambda = \{1, \dots, N\}$ . Let us for definiteness opt for a discrete time dynamics and fix the transition rates as *Metropolis rates*

$$p(\sigma, \sigma') = \begin{cases} N^{-1} \exp(-[H_\Lambda(\sigma') - H_\Lambda(\sigma)]_+), & \text{if } \|\sigma - \sigma'\|_1 = 2, \\ 0, & \text{if } \|\sigma - \sigma'\|_1 > 2, \\ 1 - \sum_{\eta \neq \sigma} p(\sigma, \eta), & \text{if } \sigma = \sigma'. \end{cases} \quad (8)$$

Now let us look at the time evolution of  $m_\Lambda(t) \equiv m_\Lambda(\sigma(t))$ . Clearly, in each step it can only increase or decrease by  $2/N$ , and one easily checks that the probability of increasing resp. decreasing depends only on the value of  $H_\Lambda$  at the starting configuration and on the number of  $-1$ 's resp.  $+1$ 's present in the configuration  $\sigma$ . But these are known once  $m_\Lambda(\sigma)$  is given. In other words,

$$\mathbb{P}[m_\Lambda(t+1) = m' | \mathcal{F}_t] = r(m_\Lambda(\sigma(t)), m') \quad (9)$$

is a function of  $m_\Lambda(t)$  only. From this one deduces readily that  $m_\Lambda(t)$  is itself a Markov chain with transition rates  $r(m, m')$  on the state space

$$\Gamma_N \equiv \{-1, -1 + 2/N, \dots, 1 - 2/N, 1\}, \quad (10)$$

which is reversible with respect to the measure

$$\mathbb{Q}_{\beta, \Lambda}(m) \equiv \mu_{\beta, \Lambda}(m_\Lambda(\sigma) = m). \quad (11)$$

Now it is well known that

$$\mathbb{Q}_{\beta, \Lambda}(m) \sim \exp(-\beta N f_\beta(m)) \quad (12)$$

with

$$f_\beta(m) = -\frac{m^2}{2} + \beta^{-1} I(m), \quad (13)$$

where

$$I(m) \equiv \frac{1+m}{2} \ln(1+m) + \frac{1-m}{2} \ln(1-m) \quad (14)$$

is Cramér's entropy function.  $f_\beta$  is a double well whenever  $\beta > 1$ . Thus  $m_N(t)$  is a random walk with reversible measure (close to)  $\exp(-\beta N f_\beta(m))$  on a lattice with spacing  $2/N$  in  $[-1, 1]$ ; this is quite close to the diffusion equation of Kramers if we chose  $V(x) = \beta f_\beta(x)$  and  $\varepsilon = (\beta N)^{-1}$ . So in the dynamics of the Curie-Weiss model, Kramers' equation can be interpreted as a diffusion approximation of the actual dynamics of the magnetisation! This is definitely a strong point in favor of Kramers' ideas.

The weak point of this observation is that it is very unstable under modifications. We are using the full permutation symmetry of this special model which is necessary to ensure that  $m_\Lambda(t)$  is even a Markov process.

Let us mention that the knowledge of the behaviour of  $m_\Lambda(t)$  a priori does not answer all questions on the dynamics of  $\sigma(t)$ . This issue has been addressed quite recently by Levin et al. [27].

There are a number of generalized mean field models that permit a similar reduction to a *multi-dimensional* diffusive Markov chain, see e.g. [10].

### 3 Large deviations

The mention of the word metastability often triggers the immediate reaction to think about *large deviations*. This is undoubtedly due to the seminal work of Freidlin and Wentzell [23], that pioneered the rigorous analysis of stochastic dynamics exhibiting metastability through the use of large deviations on path space. It is also the basis of the so-called *pathwise approach* to metastability, that was initiated by Cassandro, Galves, Olivieri, and Vares [14] in 1984. The recent monograph on metastability by Olivieri and Vares [34] gives an in-depth overview from this angle.

Let us look at this in a slightly abstract way. Let us assume that we are working with a family,  $X^\varepsilon$ , of Markov processes on a state space  $\mathcal{S}$ , which we may assume to be a complete separable normed space. Let us denote by  $\Gamma$  the set of all paths,  $\gamma: [0, T] \rightarrow \mathcal{S}$ , with  $T$  arbitrary. We may naturally equip  $\Gamma$  with the supremum norm inherited from the norm on  $\mathcal{S}$ . By a large deviation principle on path space we mean that we have a non-negative, lower semi-continuous function,  $I: \Gamma \rightarrow \mathbb{R}_+$ , with compact level sets, such that for some  $\varepsilon$  small, for any set  $A \subset \Gamma$ ,

$$-\inf_{\gamma \in \text{int}A} I(\gamma) \leq \varepsilon \ln \mathbb{P}(X^\varepsilon \in A) + o(1) \leq -\inf_{\gamma \in \text{cl}A} I(\gamma) \quad (15)$$

In a way more speaking for us is the essentially equivalent formulation that for any small enough  $\delta > 0$ , and any  $\gamma \in \Gamma$ ,

$$\varepsilon \ln \mathbb{P}(\|X^\varepsilon - \gamma\| \leq \delta) = -I(\gamma) + o(1) \quad (16)$$

In the presence of such a formulation, metastability will arise if we can identify two (or more) sets  $A, B \subset \mathcal{S}$ , such that

$$\inf_{\gamma: A \rightarrow B} I(\gamma) > 0, \quad (17)$$

and

$$\inf_{\gamma: B \rightarrow A} I(\gamma) > 0, \quad (18)$$

whereas there exists paths  $\gamma: A \rightarrow A$  and  $\gamma': B \rightarrow B$ , of strictly positive length, such that

$$I(\gamma) = I(\gamma') = 0. \quad (19)$$

Here the notation  $\gamma: A \rightarrow B$  means the set of curves (of arbitrary length) that begin in  $A$  and end in  $B$ .

Clearly in such a situation one can split the state space into two parts, one containing  $A$  and the other  $B$ , such that the process will stay exponentially (in  $1/\varepsilon$ ) long in one of the parts before going to the other; this is clearly what we understand by metastable behavior. Also, the minimizer in the variational problems (17) and (18) are clearly the most likely strategies to realize the unlikely transitions, in the sense that with probability tending to one, the process conditioned to move from  $A$  to  $B$  in finite time<sup>2</sup> will do this by remaining in an arbitrarily small neighborhood of a minimizer  $\gamma$ ; if the minimizers are unique, then they represent the optimal transition strategy.

In this latter case, we may again see a confirmation of the one-dimensional model of Kramer: it suggests that we may replace the entire process by one that is confined into an arbitrarily thin, properly chosen, tube around the optimal path and obtain the same result. But there are two difficulties: first, one would have to identify this path, and second, the equivalence would hold only on the level of precision that is given by the large deviation theory.

Before commenting on this latter aspect, let us comment on the question of where a large deviation principle on path space can be expected.

### 3.1 Diffusions with small diffusivity.

The multi-dimensional analog of Kramers' equation was the main example in the original work of Wentzell and Freidlin [23]. In that case the rate function is given by

$$I(\gamma) = \frac{1}{2} \int_0^T \|\dot{\gamma}(t) - b(\gamma(t))\|^2 dt. \quad (20)$$

The rate,  $\varepsilon$ , is simply the  $\varepsilon$  from the coefficient in front of the Brownian motion. We see that zero-action curves are only those that follow the drift field,  $b$ , almost all the time. Thus the analysis of the vector field  $b$  provides the full picture of metastable states. In the case when  $b$  is the gradient of a potential function  $V$ , this analysis boils down to the analysis of the valley structure of the landscape given by  $V$ .

### 3.2 Jump processes under rescaling.

Markov jump processes with non-heavy tailed increments in finite dimensional spaces will often satisfy a large deviation principle under suitable rescaling of space and time, e.g.

$$X^\varepsilon(t) \equiv \varepsilon X_{\varepsilon^{-1}t}. \quad (21)$$

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<sup>2</sup> I am not very careful with time here. We may assume that our sets are big enough so that the optimal connecting paths do so in  $\varepsilon$ -independent time.

One may then expect a large deviation principle for  $X^\varepsilon$ , with rate function of the form

$$I(\gamma) = \int_0^T \mathcal{L}(\gamma(t), \dot{\gamma}(t)) dt. \quad (22)$$

with a certain *Lagrange function* that can be computed as a Legendre transform of the log-moment generating function of the laws of the increments of the process  $X$ . We see that the rate,  $\varepsilon$ , arises here from the rescaling of the process.

### ***3.3 Markov processes with exponentially small transition probabilities.***

Markov processes on finite state space where some transitions occur with probabilities that are exponentially small in some parameter were considered first by Freidlin and Wentzell [23] as they occur naturally as effective processes describing the jumps of a metastable systems between its metastable states (or “cycles” as they were called). They found renewed interest in the context of stochastic dynamics of Ising type models in the limit as the inverse temperature,  $\beta$ , tends to infinity. It is clear that in that case, all moves that will increase the value of the energy,  $H_\Lambda$ , will have an exponentially small probability. These models were intensely studied in recent years by various groups, such as Catoni and Cerf [15], Cerf and Ben Arous [2], and Neves and Schonmann [30, 31], Olivieri, Scoppola, den Hollander, Nardi, etc. [32, 33, 21, 20]. In this situation, individual microscopic path can realize the minimizers of the variational principles, since path entropy plays not role in comparison to the probabilities of individual paths. One should view this as a very singular and atypical situation.

### ***3.4 Large deviations by massive entropy production.***

The stochastic Ising models we said we are interested in do not fall into any of the settings above. The dimension of state space is very high, and individual paths have not only very small probability, but even very small probability to stay “close” so a prescribed path. Thus in order to get to a large deviation description, we must seriously “lump” paths together to transform entropy into probability. One way to do this we have seen at work in the Curie-Weiss model. Passing to the variables  $m_\Lambda(t) = m_\Lambda(\sigma(t))$  identifies all path that follow the same magnetisation pattern. Typically, one path in  $m$ -space will correspond to exponentially many paths in  $\sigma$ -space. Through this map we obtain a large deviation principle in the sense of our second example above. Of course in the Curie-Weiss model, all is quite simple again due to the fact that the Hamiltonian depends only on the variables  $m_\Lambda$ . In the general case, the computation of the rate function will be a far more difficult problem, to say the least.

The choice of the map used in the entropy production procedure leaves of course a lot of freedom. One can in fact think of any coarse graining method familiar from equilibrium statistical mechanics, such as block-spin averages over boxes of some “mesoscopic” size. In principle this appears robust, but hard to carry out in practice. The most impressive example where this was done remains the seminal paper [36] by Schonmann and Shlosman on the two-dimensional Ising model under Glauber dynamics.

Another class of models that have been considered in this sense are again mean field type interaction diffusions in  $\mathbb{R}^d$ . Here one considers a system of  $n$  stochastic differential equations,

$$dX_k = \sigma(X_k)dB_k + b(X_k, \nu_n(\mathbf{X}))dr, \quad (23)$$

where  $B_k$  are independent  $d$ -dimensional Brownian motions and  $\nu_n(\mathbf{X})$  is the empirical measure

$$\nu_n(\mathbf{X}) \equiv n^{-1} \sum_{k=1}^n \delta_{X_k}. \quad (24)$$

Dawson and Gärtner [18, 19, 24] proved that the trajectories of the empirical measure converge do solutions of the McKean-Vlasov equation

$$\frac{d}{dt}\mu(t) = \mathcal{L}(\mu(t))^*\mu(t), \quad (25)$$

where  $\mathcal{L}(\mu)^*$  is the adjoint generator of the diffusion equation (23) with  $\nu_n(\mathbf{X})$  replaced by  $\mu$ . They also proved a large deviation principle for the trajectories of the empirical measure and studied the metastable behaviour of the this system.

Similar results were also obtained for a class of spin systems with long range interactions by Comets [16].

## 4 Limitations of the large deviation approach and alternatives

The large deviation method is certainly very versatile and may, in principle at least, be employed in any model context. Its main drawback is the limited precision it makes available. Indeed, all physical quantities, such as escape probabilities and transition times are computed up to multiplicative errors of the form  $\exp(\pm\delta/\varepsilon)$ , with  $\delta$  arbitrarily small but independent of  $\varepsilon$ . Partly this is due to the fact that we obtain too much information: we localise the optimal path and then calculate the probability that the process follows that path, then in reality we are interested in much less, e.g. the law of an exit time. On the other hand, even in the one-dimensional case, we fail to see the fine details of the behavior of the process near the critical saddle points that are crucial for the precise behavior of the relevant probabilities.

Since we are mostly interested in reversible Markov chains, the approach via potential theory and capacity estimates presents a convenient alternative. I have pre-



sented this at length in various occasions [7, 8] and thus give just a very short sketch of the key elements here.

I consider a general Markov chain (in discrete time for definiteness) with discrete state space  $\mathcal{S}$  and transition matrix  $P$ . I like to call  $P - \mathbb{1} \equiv L$  the generator. Note that the entire formalism carries over (under some suitable regularity conditions) to the continuous setting, of course.

For two disjoint sets  $A, B \subset \mathcal{S}$ , the equilibrium potential,  $h_{A,B}$ , is the harmonic function, i.e. the solution of the equation

$$(Lh_{A,B})(\sigma) = 0, \quad \sigma \notin A \cup B, \quad (26)$$

with boundary conditions

$$h_{A,B}(\sigma) = \begin{cases} 1, & \text{if } \sigma \in A \\ 0, & \text{if } \sigma \in B \end{cases}. \quad (27)$$

The *equilibrium measure* is the function

$$e_{A,B}(\sigma) \equiv -(Lh_{A,B})(\sigma) = (Lh_{B,A})(\sigma), \quad (28)$$

which clearly is non-vanishing only on  $A$  and  $B$ . The capacity,  $\text{cap}(A, B)$  is defined as

$$\text{cap}(A, B) \equiv \sum_{\sigma \in A} \mu(\sigma) e_{A,B}(\sigma). \quad (29)$$

By the discrete analog of the first Green's identity, we get that alternatively,

$$\text{cap}(A, B) = \frac{1}{2} \sum_{\sigma, \sigma' \in \mathcal{S}} \mu(\sigma) p(\sigma, \sigma') [h_{A,B}(\sigma) - h_{A,B}(\sigma')]^2 = \Phi(h_{A,B}), \quad (30)$$

where the right-hand side is The functional appearing on the left-hand sides of these relations is called the *Dirichlet form* or *energy*. As a consequence of the *maximum principle*, the function  $h_{A,B}$  is the unique minimizer of  $\Phi$  with boundary conditions (27), which implies the *Dirichlet principle*:

$$\text{cap}(A, B) = \inf_{h \in \mathcal{H}_{A,B}} \Phi(h), \quad (31)$$

where  $\mathcal{H}_{A,B}$  denotes the space of functions satisfying (27).

An important observation is that equilibrium potentials and equilibrium measures also determine the Green's function. In fact (see e.g. [11, 8]),

$$h_{A,B}(\sigma) = \sum_{\sigma' \in A} G_{\mathcal{S} \setminus B}(\sigma, \sigma') e_{A,B}(\sigma') \quad (32)$$

(32) can be used to give the following representation for mean hitting times

$$\sum_{\sigma \in A} \mu(\sigma) e_{A,B}(\sigma) \mathbb{E}_\sigma \tau_B = \sum_{\sigma' \in \mathcal{S}} \mu(\sigma') h_{A,B}(\sigma'), \quad (33)$$

or, after normalizing the left-hand side to be an expectation,

$$\mathbb{E}_{V_{A,B}} \tau_B = \frac{1}{\text{cap}(A,B)} \sum_{\sigma' \in S} \mu(\sigma') h_{A,B}(\sigma'). \quad (34)$$

The point to retain for us is that estimates in hitting times can be obtained once we have control over capacities and the equilibrium potential. Note that of course, knowing the equilibrium potential alone is good enough, since we can get the capacity by just plugging it into the Dirichlet form. The point, however, is that it is easier to estimate the capacity than to find the equilibrium potential: we will see why.

Note that computing the equilibrium potential amounts to solving a boundary value problem for a finite difference operator, which is the discrete analogue of solving a boundary value problem for an elliptic pde. The only case when this is easily doable is when  $\mathcal{S}$  has the structure of a one-dimensional set and the transition matrix connects only nearest neighbors. In that case equation (26) can be solved by recursion and we obtain an explicit solution in terms of a sum. This is analogous to the case of a one-dimensional diffusion, where we can solve the boundary value problem in terms of an explicit integral. This is the second important fact that we will keep in mind.

## 5 Capacity estimates

The first pleasant surprise is that the Dirichlet principle is perfectly suited for the idea of (imperfect) lumping or coarse graining. Let  $m$  map  $\mathcal{S}$  to some lower dimensional space,  $\Gamma$ . Let us for simplicity assume that two sets  $A, B$  are adapted to the map  $m$  in the sense that  $A = m^{-1}(m(A))$ , and likewise for  $B$ .

Then we have the following obvious bound:

$$\begin{aligned} \text{cap}(A,B) &= \inf_{h \in \mathcal{H}_{A,B}} \frac{1}{2} \sum_{\sigma, \sigma' \in \mathcal{S}} \mu(\sigma) p(\sigma, \sigma') [h(\sigma) - h(\sigma')]^2 \\ &\leq \inf_{u \in \mathcal{G}_{m(A), m(B)}} \frac{1}{2} \sum_{\sigma, \sigma' \in \mathcal{S}} \mu(\sigma) p(\sigma, \sigma') [u(m(\sigma)) - u(m(\sigma'))]^2 \\ &= \inf_{u \in \mathcal{G}_{m(A), m(B)}} \frac{1}{2} \sum_{x, x' \in \Gamma} [u(x) - u(x')]^2 \sum_{\sigma \in m^{-1}(x)} \mu(\sigma) \sum_{\sigma' \in m^{-1}(x')} p(\sigma, \sigma') \\ &\equiv \inf_{u \in \mathcal{G}_{m(A), m(B)}} \frac{1}{2} \sum_{x, x' \in \Gamma} \mathcal{Q}(x) r(x, x') [u(x) - u(x')]^2 \\ &\equiv \text{CAP}(m(A), m(B)). \end{aligned} \quad (35)$$

with

$$r(x, x') \equiv \frac{1}{\mathcal{Q}_{\beta, N}[\omega](\mathbf{x})} \sum_{\sigma \in m^{-1}(x)} \mu(\sigma) \sum_{\sigma' \in m^{-1}(x')} p(\sigma, \sigma'). \quad (36)$$

Here

$$\mathcal{H}_{A, B} \equiv \{h : S \rightarrow [0, 1] : \forall \sigma \in A, h(\sigma) = 1, \forall \sigma \in B, h(\sigma) = 0\} \quad (37)$$

and

$$\mathcal{G}_{m(A), m(B)} \equiv \{u : \Gamma \rightarrow [0, 1] : \forall x \in m(A), u(x) = 1, \forall x \in m(B), u(x) = 0\}. \quad (38)$$

Thus the map introduces always new transition rates and a new Dirichlet form, thus a new, “lumped”, Markov process. Equality in the above relation holds if and only if the equilibrium potential corresponding to the original chain is in fact a function of the new variables  $m$  only. This is exactly the case when lumping in the original sense works, i.e. when the image of the chain under the map  $m$  is Markov.

But note now that we are in a much better shape as before. In particular, we understand that the quality of the upper bound will not depend on the global quality of the approximation of the equilibrium potential by a function depending only on  $m(\sigma)$ , but only on the quality of this approximation in the region of phase space where the main contribution to the capacity is expected to come from. In practice, we tend to believe that the best way to get a good estimate for the capacity is to find a good mapping,  $m$ , and then to find an almost optimal solution for the new Dirichlet form. Of course, to justify such a believe, we must in the end have a way to prove a lower bound.

### 5.1 Random path representation and lower bounds on capacities.

The canonical way to get lower bounds on capacities, first exploited in [6] and then in [9], is to exploit a dual variational representation of capacities in terms of flows, due to Berman and Konsowa [4].

It will be convenient to think of the quantities  $\mu(\sigma)p_N(\sigma, \sigma')$  as *conductances*,  $c(\sigma, \sigma')$ , associated to the edges  $e = (\sigma, \sigma')$  of the graph of allowed transitions of our dynamics.

**Definition 1.** Given two disjoint sets,  $A, B \subset S$ , a non-negative, cycle free *unit flow*,  $f$ , from  $A$  to  $B$  is a function  $f : \mathcal{E} \rightarrow \mathbb{R}_+ \cup \{0\}$ , such that the following conditions are verified:

- (i) if  $f(e) > 0$ , then  $f(-e) = 0$ ;
- (ii)  $f$  satisfies *Kirchoff's law*, i.e. for any vertex  $a \in S \setminus (A \cup B)$ ,

$$\sum_b f(b, a) = \sum_d f(a, d); \quad (39)$$

- (iii)

$$\sum_{a \in A} \sum_b f(a, b) = 1 = \sum_a \sum_{b \in B} f(a, b); \quad (40)$$

(iv) any path,  $\gamma$ , from  $A$  to  $B$  such that  $f(e) > 0$  for all  $e \in \gamma$ , is self-avoiding.

We denote the space of non-negative, cycle free unit flows from  $A$  to  $B$  by  $\mathbb{U}_{A,B}$ .

An important unit flow is the *harmonic flow*, associated to the equilibrium potential,  $h_{A,B}$ . It is defined as

$$f^*(a,b) \equiv \frac{1}{\text{cap}(A,B)} c(a,b) (h_{A,B}(a) - h_{A,B}(b))_+. \quad (41)$$

One can easily verify, using that  $h_{A,B}$  is a harmonic function,  $f^*$  is a non-negative unit flow.

The key observation is that any  $f \in \mathbb{U}_{A,B}$  gives rise to a *lower bound* on the capacity  $\text{cap}(A,B)$ , and that this bound becomes sharp for the harmonic flow. To see this we construct from  $f$  a stopped Markov chain  $\mathbb{X} = (\mathbb{X}_0, \dots, \mathbb{X}_\tau)$  as follows: For each  $a \in S \setminus B$  define  $F(a) = \sum_b f(a,b)$ .

We define the initial distribution of our chain as  $\mathbb{P}^f(a) = F(a)$ , for  $a \in A$ , and zero otherwise. The transition probabilities are given by

$$q^f(a,b) = \frac{f(a,b)}{F(a)}, \quad (42)$$

for  $a \notin B$ , and the chain is stopped on arrival in  $B$ .

Thus, given a trajectory  $\mathcal{X} = (a_0, a_1, \dots, a_r)$  with  $a_0 \in A$ ,  $a_r \in B$  and  $a_\ell \in S \setminus (A \cup B)$  for  $\ell = 0, \dots, r-1$ ,

$$\mathbb{P}^f(\mathbb{X} = \mathcal{X}) = \frac{\prod_{\ell=0}^{r-1} f(e_\ell)}{\prod_{\ell=0}^{r-1} F(a_\ell)}, \quad (43)$$

where  $e_\ell = (a_\ell, a_{\ell+1})$  and we use the convention  $0/0 = 0$ . Note that, with the above definitions, the probability that  $\mathbb{X}$  passes through an edge  $e$  is

$$\mathbb{P}^f(e \in \mathbb{X}) = \sum_{\mathcal{X}} \mathbb{P}^f(\mathcal{X}) \mathbb{1}_{\{e \in \mathcal{X}\}} = f(e). \quad (44)$$

Consequently, we have a partition of unity,

$$\mathbb{1}_{\{f(e) > 0\}} = \sum_{\mathcal{X}} \frac{\mathbb{P}^f(\mathcal{X}) \mathbb{1}_{\{e \in \mathcal{X}\}}}{f(e)}. \quad (45)$$

We are ready now to derive our  $f$ -induced lower bound: For every function  $h$  with  $h|_A = 0$  and  $h|_B = 1$ ,

$$\begin{aligned} \frac{1}{2} \sum_e c(e) (\nabla_e h)^2 &\geq \sum_{e: f(e) > 0} c(e) (\nabla_e h)^2 \\ &= \sum_{\mathcal{X}} \sum_{e \in \mathcal{X}} \mathbb{P}^f(\mathcal{X}) \frac{c(e)}{f(e)} (\nabla_e h)^2. \end{aligned}$$

As a result, interchanging the minimum and the sum,

$$\begin{aligned} \text{cap}(A, B) &\geq \sum_r \sum_{\mathcal{X}=(a_0, \dots, a_r)} \mathbb{P}^f(\mathcal{X}) \min_{h(a_0)=0, h(a_r)=1} \sum_0^{r-1} \frac{c(a_\ell, a_{\ell+1})}{f(a_\ell, a_{\ell+1})} (h(a_{\ell+1}) - h(a_\ell))^2 \\ &= \sum_{\mathcal{X}} \mathbb{P}^f(\mathcal{X}) \left[ \sum_{e \in \mathcal{X}} \frac{f(e)}{c(e)} \right]^{-1}. \end{aligned} \quad (46)$$

Since for the equilibrium flow,  $f^*$ ,

$$\sum_{e \in \mathcal{X}} \frac{f^*(e)}{c(e)} = \frac{1}{\text{cap}(A, B)}, \quad (47)$$

with  $\mathbb{P}^{f^*}$ -probability one, the bound (46) is sharp.

Thus we have proven the following result from [4]:

**Proposition 1.** *Let  $A, B \subset S$ . Then, with the notation introduced above,*

$$\text{cap}(A, B) = \sup_{f \in \mathbb{U}_{A, B}} \mathbb{E}^f \left[ \sum_{e \in \mathcal{X}} \frac{f(e)}{c(e)} \right]^{-1} \quad (48)$$

One should note that the rather intricate character of the lower bound through these flows is particular to the discrete graph structure of discrete models. In the case of diffusions, this trivialises to the replacement of gradients by optimally chosen directional derivatives in the Dirichlet form.

So these are our basic tools. The next step is to show that all will work on the level of the mesoscopic approximations.

## 5.2 Capacity estimates for mesoscopic chains and the return of $d = 1$ .

We have said before that we believe that by choosing good coarse grainings we will get good upper bounds. We can make this more precise: under reasonable assumptions, we can find optimal upper bounds amongst the class of test-functions that depend only on the coarse grained variables.

Now we must be more specific. We will assume that our coarse graining goes through functions

$$m : \mathcal{S}_\Lambda \rightarrow \Gamma \subset \mathbb{R}^n \quad (49)$$

where in principle we may allow  $n$  to depend on  $\Lambda$ .

We will also assume that the induced equilibrium measure on  $m$ ,

$$\mathbb{Q}(m) \equiv \mu \circ m^{-1}, \quad (50)$$

will be of the form

$$\mathbb{Q}(m) \sim \exp(-NF_\Lambda(m)), \quad (51)$$

where of course  $F_\Lambda$  depends on everything, but is of order unity. Computing  $F$  will be hard problem in equilibrium statistical mechanics, well known from the theory of renormalisation. There are instances, however, when this has been achieved completely [26]. The parameter  $N$  can be made large depending on the choice of the coarse graining (in fact it corresponds to the volume of blocks in the case of block spin variables).

On the level of such a *mesoscopic* description, metastable states correspond to local minima of the function  $F$ . One will then expect that the essential contributions from the Dirichlet form small neighborhoods of the *essential saddle* points over which two such minima can be connected. Saddle points may in some cases be numerous, in particular if they correspond to localised structures which then, by symmetry, may entail volume factors.

Basically, we expect to be able to identify a neighborhood,  $D$ , of the essential saddle points with the following properties:

- (i)  $F$  is well approximated by a quadratic<sup>3</sup> function,  $\hat{F}$ , on  $D$ , in the sense that on  $B$ ,  $|F(m) - \hat{F}(m)| = o(1/N)$ .
- (ii) The contributions from  $D^c$  to the Dirichlet form can be neglected.

The latter request may sound strange: for part of the complement of  $D$ , one may be able to show this simply because the integral over  $\exp(-NF)$  becomes negligible. However this only concerns the region where  $F(m) > F(z^*)$  ( $F(z^*)$  being the value of  $F$  at the saddle). To control the rest, we must effectively know that the harmonic potential is almost a constant.

Let us postpone the discussion how point (ii) can be verified for a moment. The first point to note is that, if  $\hat{F}$  is quadratic, with possibly some zero-eigenvalues corresponding to symmetries, we should expect that  $D$  extends in the directions of non-zero eigenvalues by something of order  $N^{-1/2} \ln N$ . This means that under plausible continuity assumptions on the transition rates  $r(m, m')$ , we can assume that without introducing significant errors, we can replace the Dirichlet form on  $D$  by the simplified one (assuming also the rates are such that only one coordinate can be changed by an amount of order  $1/N$ , which is reasonable if they are derived from Glauber dynamics),

$$\hat{\Phi}(h) \equiv \sum_m \sum_{\ell=1}^n r_\ell \exp\left(-\frac{N}{2}(m, Am)\right) [h(m + e_\ell/N) - h(m)]^2. \quad (52)$$

This, on the other hand is very close to its continuum approximation,

$$\tilde{\Phi}(h) \equiv \int \exp\left(-\frac{N}{2}(x, Ax)\right) (\nabla h(x), \nabla h(x))_r dx, \quad (53)$$

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<sup>3</sup> This may be general forms, see [3] for examples.

where  $(f, g)_r \equiv \sum_{\ell=1}^n f_\ell g_\ell r_\ell$ . The point is that for such a functional, one can readily find a family of harmonic functions. Namely, a harmonic function for (53) solves

$$\sum_{\ell} r_{\ell} (\partial_{\ell} h(x) - (e_{\ell}, Ax) \partial_{\ell} h(x)) = 0. \quad (54)$$

Now let  $f(t)$  be a solution of  $f'' - \gamma N_t f' = 0$ . Set  $h(x) = f((x, v))$ , for some vector  $v$ . Inserting this ansatz into (54) yields

$$\sum_{\ell} r_{\ell} v_{\ell} (v_{\ell} \gamma(x, v) - (e_{\ell}, Ax)) = 0. \quad (55)$$

In the case  $r_{\ell} = 1$ , we see that this is satisfied if  $v$  is an eigenvector of  $A$  with eigenvalue  $\gamma$ ; in the general case,  $v$  should satisfy

$$r_{\ell} \sum_k A_{\ell k} v_k = \gamma v_{\ell}. \quad (56)$$

The point is that the solutions of this equation form an orthonormal basis for the inner product  $(\cdot, \cdot)_r$ . Choosing such a vector with negative  $\gamma$  (this will be unique), we can construct  $f$  that goes from 0 to 1. Using this, to construct a sufficiently good approximation to the minimizer everywhere to get the desired bound on the capacity is just patchwork.

This is basically good news. On the level of the mesoscopic model, we can expect to get sharp results. Thus we may hope to get to sharp estimates for the full model by just refining the coarse graining. The only non-trivial example so far where this programme has been pushed through and shown to be successful is the Random Field Curie Weiss model [6]. The problems in verifying the result lies in the application of the Berman Konsowa principle, i.e. in the construction of an optimal flow for the lower bound. We do not yet have a canonical way of doing this and this is clearly still place where more work will be needed.

## 6 Stochastic partial differential equations

From the point of view of the discussion before, a natural class of intermediate models to study are stochastic partial differential equations, to be seen e.g. as heuristic diffusion limits of block spin approximations. However, spde's with small noise arise in any other modeling contexts and are certainly interesting models in their own right.

The simplest spde of interest is the stochastic Allen-Cahn equation,

$$dX(x, t) = \frac{\gamma}{4\pi^2} \Delta X(x, t) dt - \nabla f(X(x, t)) dt + \sqrt{2\epsilon} dB(x, t) \quad (57)$$

with  $x \in D \subset \mathbb{R}^d$  and  $t \in \mathbb{R}_+$ .  $f$  is a double well potential,

$$f(s) = \frac{x^4}{4} - \frac{x^2}{2}. \quad (58)$$

In the case when  $d = 1$ , the noise term  $B$  can be chosen as space-time white noise. It is well-known that in that case this equation admits classical solutions [17]. In higher dimensions this is not the case, and some regularisation of the noise term is needed.

Eq. (57) arises as the limit of a system of ordinary stochastic differential equations (for simplicity we write only the case of one spatial dimension)

$$dX^N(t) = -\nabla F_{\gamma,N}(X^N(t))dt + \sqrt{2\varepsilon}dB^N(t) \quad (59)$$

where  $B^N(t)$  is an  $N$ -dimensional vector of Brownian motions and

$$F_{\gamma,N}(X) = \frac{1}{N} \sum_{i \in \Lambda_N} \left( \frac{1}{4}X_i^4 - \frac{1}{2}X_i^2 + N^2 \frac{\gamma}{2\pi^2} (X_{i+1} - X_i)^2 \right) \quad (60)$$

Then  $\widehat{X}^N(x, t) = X_i^N(tN)$ , for  $x \in [i/N, (i+1)/N)$  converges to a solution of (57), as  $N$  goes to zero.

For any finite  $N$ , one can now use the results of [12] and obtain precise formulae for the mean hitting time of e.g. a neighborhood of the minimum  $X \equiv 1$  when starting from  $X \equiv -1$ . In the simpler case, when  $\gamma > 1$ , there are only three critical points  $\pm 1$  and the saddle 0, and one gets (see [1])

$$\mathbb{E}_{-1}[\tau_{B_+}] = \frac{2\pi e^{\frac{N}{4\varepsilon}} \sqrt{|\det(\nabla^2 F_{\gamma,N}(O))|}}{\sqrt{\det(\nabla^2 F_{\gamma,N}(-1))}} (1 + O(\sqrt{\varepsilon} |\ln \varepsilon|^3)). \quad (61)$$

The determinants can be computed explicitly and one gets

$$\frac{\sqrt{|\det(\nabla^2 F_{\gamma,N}(O))|}}{\sqrt{\det(\nabla^2 F_{\gamma,N}(I_-))}} = \left[ 1 - \frac{3}{2+2\gamma} \right]^{\frac{e(N)}{2}} \prod_{k=1}^{\lfloor \frac{N-1}{2} \rfloor} \left[ \frac{\gamma N^2 \sinh^2(k\pi/N)/\pi^2 - 1}{\gamma N^2 \sinh^2(k\pi/N)/\pi^2 + 2} \right] \quad (62)$$

where  $e(N) = 1$  if  $N$  is even and 0 if  $N$  is odd. One readily sees that this latter expression converges, as it should, to

$$V(\mu) = \prod_{k=1}^{+\infty} \left[ \frac{\gamma k^2 - 1}{\gamma k^2 + 2} \right] \quad (63)$$

This fact will be quite general and holds also for smaller values of  $\gamma$ , see e.g. [28].

The main issue it thus to prove the uniformity of the error estimates in  $N$ . This may look difficult in view of our discussion above on capacity estimates, which required uniformly good quadratic approximations on a neighborhood of the saddle point. The point is, however, that the second derivative of the function  $F_{\gamma,N}$  as an operator has eigenvalues of order  $k^2$ . Hence the invariant measure concentrates very rapidly in the directions of the higher eigenvalues, making the problem *effectively* finite dimensional.



## 7 Open issues

To conclude this brief review, let me mention some of the open issues that I feel need to be addressed in the coming years.

### 7.1 Initial distributions and regularity theory

The key equation linking capacities to physical quantities is (34). While as an equation it is perfectly true, it is useful only if the sets  $A, B$  are chosen “not too small”. Otherwise, both numerator and denominator will be excessively small, and the calculation of the ratio becomes an issue of subtle second order corrections, which will in most situations be next to impossible to achieve.

In many examples, this does not cause too much of a problem. Functions such as  $\mathbb{E}_x \tau_B$  should be relatively constant on “small” sets  $A$  of interest. This can be proven either by analytic means (see [12] using Hölder estimates in the setting of diffusion processes, or coupling arguments, see [29] for the case of stochastic (partial) differential equations, or [5] for a stochastic spin system. In the last case, the absence of contracting drifts on the level of the microscopic variables made the analysis already rather cumbersome and rather model dependent. It would clearly be desirable to have more universally applicable tools at our disposal.

A similar issue arises in the context of spectral theory. In a number of contexts (finite dimensional diffusions [13], (essentially) finite state space [11]), there is a very sharp link between metastable states and small eigenvalues of the generator. One would clearly expect this to be true in much more generality. The method used in [13], essentially an application of an old idea of Wentzell [37, 38] is again based on regularity properties, this time of eigenfunction of the generator. One should again expect this to be true in more generality, but a good theory seems to be missing so far.

### 7.2 Canonical constructions of flows

In [6] we have proven a lower bound on capacities by constructing a specific *microscopic flow* for the Berman-Konsowa principle. The fact that this worked out well was due to self-averaging resp. homogenization effects, and both the construction and the proofs relied quite heavily on specific properties of the model. Whenever we want to control a model of microscopic spin- or particle dynamics, we will have to be able to do the same. Is there some generic way of doing and proving this? This is clearly one of the most pressing issues to be resolved in the coming years.

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