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Metastable states, quasi-stationary distributions and soft measures[☆]

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Abstract

We establish metastability in the sense of Lebowitz and Penrose under practical and simple hypotheses for Markov chains on a finite configuration space in some asymptotic regime. By comparing restricted ensembles and quasi-stationary measures, and introducing soft measures as an interpolation between the two, we prove an asymptotic exponential exit law and, on a generally different time scale, an asymptotic exponential transition law. By using potential-theoretic tools, and introducing "(κ, λ)-capacities", we give sharp estimates on relaxation time, as well as mean exit time and transition time. We also establish local thermalization on shorter time scales.

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1. Metastability after Lebowitz and Penrose

1.1. Phenomenology and modelization

Lebowitz and Penrose characterized *metastable thermodynamic states* by the following properties [41]:

(a) only one thermodynamic phase is present,
(b) a system that starts in this state is likely to take a long time to get out,
(c) once the system has gotten out, it is unlikely to return.

We can think, for example, about freezing fog made of small droplets in which only one phase is present (liquid phase) that remains for a long time in such a state (until collision with ground or trees, forming then hard rime) and that once frozen will typically not return to liquid state before pressure or temperature has changed.

To model such a state they considered in [41] a deterministic dynamics with equilibrium measure μ. First, they associated with the metastable phase a subset $\mathcal{R}$ of the configuration space, and described this metastable state by the *restricted ensemble* $\mu_{\mathcal{R}} = \mu(\cdot|\mathcal{R})$. Second, they proved that the escape rate from $\mathcal{R}$ of the system started in $\mu_{\mathcal{R}}$ is maximal at time $t = 0$, and that this initial escape rate is very small. Last, they used standard methods of equilibrium statistical mechanics to deal with (c). As an estimate of the returning probability to the metastable state they used the fraction of members of the *equilibrium* ensemble that have configurations in $\mathcal{R}$ and they noted [41, Section 8]:

> This amounts to assuming that a system whose dynamical state has just left $\mathcal{R}$ is no more likely to return to it than one whose dynamical state was never anywhere near $\mathcal{R}$. The validity of this assumption, at least in the short run, is dubious, but at least it provides us with some indication of what to expect.

In this paper we want to give a different model for the same phenomenology that overcomes the last difficulty. We will work with stochastic processes rather than deterministic dynamics, but the Lebowitz–Penrose modelization will be our guideline. We will try to recover this phenomenology under simple and practical hypotheses only. Since the study of metastability has been considerably enriched after the Lebowitz and Penrose work, we want also to incorporate in our modelling as much as possible of what was previously achieved. We will then make a brief and partial review of these achievements. Our goals and starting ideas will depend on this review but not our proofs, since we want to make this paper as self-contained as possible. Our model and results are presented in Section 2. Examples of applications are given in Section 7.

1.2. A partial review

Since the Lebowitz and Penrose paper, an enormous amount of work has been done to describe the metastability phenomenon. In particular Cassandro, Galves, Olivieri and Vares introduced the path-wise approach, which focused, in the context of stochastic processes, on time averages associated with an asymptotic exponential law [19]. This was further developed by the pioneering works of Neves and Schonmann who studied the typical paths for stochastic Ising model in a given volume in the low temperature regime [37,38]. This work was then extended to higher dimensions, infinite-volume and fixed-temperature regimes, locally conservative dynamics and probabilistic cellular automata [23,7,43,28,21,20].